Pentaarylfullerenes as noncoordinating cyclopentadienyl anions

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# CIF-file generated for C121H87LiO4                  P21/n         q1281
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2008-09-24 # Formatted by publCIF
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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Inorg. Chem.'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2008-08-24  14:09:20


 Consider this CIF submission for deposition of the (first)
 X-ray structure of a manuscript to be submitted to : Inorg. Chem.
  (Our Compound_Identification_Code : q1281)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)
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# 3. TITLE AND AUTHOR LIST

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.

# The loop structure below should contain the names and adresses of all
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'?' # author name
;   # author related footnote
;
;   # Address of this author
;
   'Meetsma, Auke'
;
```

```
 ? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

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# 4. TEXT

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_publ_section_exptl_prep
;

;
_publ_section_exptl_refinement
;
The asymmetric unit consists of two moieties: a Li-THF complex and bucky ball
complex.

The scattering power of the crystals investigated was very weak: nearby an half
of the unique (till \q 24.11 \% merged reflections obey the <i>F~o~</i> * 4.0
*(<i>F~o~</i>) criterion of observability. This implies that the mean s.u. is
large compared to the mean magnitude of the (even more than double of the
squared) structure factor.

The hydrogen atoms were generated by geometrical considerations, constrained to
idealized geometries, and allowed to ride on the carrier atoms with an
isotropic displacement parameter related to the equivalent displacement
parameter of their carrier atoms, with <i>U</i>~iso~(H) = 1.2<i>U</i>~eq~(C)
or 1.5<i>U</i>~eq~(methyl C). The methyl-groups were refined as rigid groups,
which were allowed to rotate free. Assigned values of bond distances:
secondary C---H~2~ = 0.99 \%A, methyl C---H~3~ = 0.98 \%A and aromatic C---H =
0.95 \%A.
;


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;

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Allen, F. H. (2002). Acta Cryst. B58, 380--388.

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;

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Fig. 1. Perspective PLUTO drawings of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.
;

_publ_section_acknowledgements
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(type here to add acknowledgements)
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5. CHEMICAL DATA

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;
;
_chemical_name_common ?

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_chemical_formula_moiety
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# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural         ?
_chemical_formula_sum
'C121 H87 Li O4'
_chemical_formula_iupac              ?
_chemical_formula_weight               1611.96
_chemical_compound_source           'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 O   O    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Li  Li   -0.0003    0.0001
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
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 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==============================================================================

# 6. CRYSTAL DATA

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_symmetry_space_group_name_H-M       'P 21/n'
_symmetry_Int_Tables_number                14

loop_
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_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 1/2-x,1/2+y,1/2-z
   3 -x,-y,-z
   4 1/2+x,1/2-y,1/2+z

_cell_length_a                         14.3757(14)
_cell_length_b                         18.0389(18)
_cell_length_c                         30.883(3)
_cell_angle_alpha                      90
_cell_angle_beta                       91.0674(16)
_cell_angle_gamma                      90
_cell_volume                          8007.3(14)
_cell_formula_units_Z                  4

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      9980
_cell_measurement_theta_min        2.46
_cell_measurement_theta_max       26.33
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   9980 reflections after integration using the SAINTPLUS
   software package (Bruker, 2000).
```

```
 Reduced cell calculations did not indicate any higher metric lattice symmetry
   and examination of the finalatomic coordinates of the structure did not
   yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description      'block'
_exptl_crystal_colour            'red'
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_exptl_crystal_size_min           0.22
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_exptl_crystal_density_meas       ?
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_exptl_absorpt_coefficient_mu     0.079
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_exptl_absorpt_correction_T_max    0.9828

#===============================================================================

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_diffrn_radiation_wavelength           0.71073
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_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method           '\f and \w scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
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;
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_diffrn_standards_interval_time      .
_diffrn_standards_decay_%            0

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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
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_diffrn_reflns_av_sigmaI/netI      0.1155
_diffrn_reflns_limit_h_min         -16
_diffrn_reflns_limit_h_max         16
_diffrn_reflns_limit_k_min         -20
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_diffrn_reflns_limit_l_min         -35
_diffrn_reflns_limit_l_max         35
_diffrn_reflns_theta_min           2.46
_diffrn_reflns_theta_max           24.11
_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              24.11
_diffrn_measured_fraction_theta_full   0.998

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT-Plus & SADABS (Bruker, 2006).
;

# number of unique reflections
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_reflns_number_gt                  6269
_reflns_threshold_expression     I>2\s(I)


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_computing_cell_refinement          'SAINT-Plus, Version 6.45, (Bruker, 2006)'
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_computing_structure_solution
;
 SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLATON (Spek, 2003)
 PLUTO (Meetsma, 2007)
;
_computing_publication_material      'PLATON (Spek, 2003)'

#=============================================================================

# 8. REFINEMENT DATA


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
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_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration '.'

_refine_ls_abs_structure_Flack   ?
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_refine_ls_number_parameters     1140
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_refine_ls_number_constraints    ?
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_refine_ls_R_factor_gt           0.0617
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_refine_ls_wR_factor_gt          0.1517
_refine_ls_goodness_of_fit_ref   0.896
_refine_ls_restrained_S_all      0.896
_refine_ls_shift/su_max          0.000
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_atom_site_fract_z
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_atom_site_refinement_flags
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O12 O Uani 0.65481(19) 0.11181(15) 0.32454(9) 1.000 0.0529(11) . .
O13 O Uani 0.4710(2) 0.12666(18) 0.37179(9) 1.000 0.0584(11) . .
O14 O Uani 0.6102(2) 0.2680(2) 0.36603(10) 1.000 0.0740(14) . .
C11 C Uani 0.4402(3) 0.2801(3) 0.28901(15) 1.000 0.0667(19) . .
C12 C Uani 0.3702(3) 0.2594(3) 0.25530(15) 1.000 0.0675(19) . .
C13 C Uani 0.4254(3) 0.2181(2) 0.22090(13) 1.000 0.0441(17) . .
C14 C Uani 0.5193(3) 0.2022(2) 0.24231(12) 1.000 0.0427(16) . .
C15 C Uani 0.7386(3) 0.1320(2) 0.30400(14) 1.000 0.0507(17) . .
C16 C Uani 0.8163(3) 0.0924(3) 0.32631(16) 1.000 0.0645(19) . .
C17 C Uani 0.7694(3) 0.0392(3) 0.35775(14) 1.000 0.0539(17) . .
```

```
C18 C Uani 0.6714(3) 0.0386(3) 0.34140(15) 1.000 0.0596(17) . .
C19 C Uani 0.4540(3) 0.1266(3) 0.41716(13) 1.000 0.0519(17) . .
C110 C Uani 0.3842(3) 0.0657(3) 0.42487(16) 1.000 0.068(2) . .
C111 C Uani 0.3318(3) 0.0612(3) 0.38174(18) 1.000 0.070(2) . .
C112 C Uani 0.4036(4) 0.0821(4) 0.34990(18) 1.000 0.092(3) . .
C113 C Uani 0.6572(4) 0.3271(3) 0.34220(17) 1.000 0.072(2) . .
C114 C Uani 0.7559(5) 0.3276(3) 0.3584(2) 1.000 0.108(3) . .
C115 C Uani 0.7437(8) 0.2949(5) 0.4034(3) 1.000 0.234(6) . .
C116 C Uani 0.6540(5) 0.2683(5) 0.40783(18) 1.000 0.132(4) . .
Li1 Li Uani 0.5601(5) 0.1804(5) 0.3393(2) 1.000 0.059(3) . .


H11 H Uiso 0.46852 0.32870 0.28247 1.000 0.0801 . .
H11' H Uiso 0.41165 0.28242 0.31791 1.000 0.0801 . .
H12 H Uiso 0.34003 0.30404 0.24282 1.000 0.0809 . .
H12' H Uiso 0.32168 0.22693 0.26752 1.000 0.0809 . .
H13 H Uiso 0.39372 0.17135 0.21247 1.000 0.0529 . .
H13' H Uiso 0.43272 0.24913 0.19476 1.000 0.0529 . .
H14 H Uiso 0.53575 0.14914 0.23929 1.000 0.0512 . .
H14' H Uiso 0.56859 0.23254 0.22909 1.000 0.0512 . .
H15 H Uiso 0.74822 0.18625 0.30599 1.000 0.0606 . .
H15' H Uiso 0.73564 0.11795 0.27302 1.000 0.0606 . .
H16 H Uiso 0.85712 0.12775 0.34217 1.000 0.0774 . .
H16' H Uiso 0.85402 0.06476 0.30523 1.000 0.0774 . .
H17 H Uiso 0.79742 -0.01091 0.35648 1.000 0.0643 . .
H17' H Uiso 0.77367 0.05777 0.38788 1.000 0.0643 . .
H18 H Uiso 0.66290 0.00088 0.31836 1.000 0.0711 . .
H18' H Uiso 0.62826 0.02738 0.36514 1.000 0.0711 . .
H19 H Uiso 0.42866 0.17508 0.42627 1.000 0.0623 . .
H19' H Uiso 0.51229 0.11698 0.43376 1.000 0.0623 . .
H110 H Uiso 0.34191 0.07872 0.44864 1.000 0.0811 . .
H110' H Uiso 0.41558 0.01819 0.43186 1.000 0.0811 . .
H111 H Uiso 0.30832 0.01037 0.37626 1.000 0.0844 . .
H111' H Uiso 0.27882 0.09625 0.38077 1.000 0.0844 . .
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H112' H Uiso 0.37469 0.11016 0.32560 1.000 0.1102 . .
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H114' H Uiso 0.79617 0.29611 0.34037 1.000 0.1295 . .
H115 H Uiso 0.78872 0.25410 0.40815 1.000 0.2810 . .
H115' H Uiso 0.75628 0.33355 0.42556 1.000 0.2810 . .
H116 H Uiso 0.61896 0.30046 0.42775 1.000 0.1582 . .
H116' H Uiso 0.65559 0.21751 0.41993 1.000 0.1582 . .


C21 C Uani 0.7906(2) 0.14556(19) 0.07214(10) 1.000 0.0229(11) . .
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C24 C Uani 0.7746(2) 0.24443(19) 0.11732(11) 1.000 0.0233(12) . .
C25 C Uani 0.7640(2) 0.16688(19) 0.11435(11) 1.000 0.0239(11) . .
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C27 C Uani 0.8762(2) 0.20921(19) 0.00967(11) 1.000 0.0267(12) . .
C28 C Uani 0.8537(2) 0.34498(19) 0.07134(11) 1.000 0.0250(12) . .
C29 C Uani 0.7827(2) 0.28677(19) 0.15937(11) 1.000 0.0252(11) . .
C210 C Uani 0.7626(2) 0.11480(19) 0.15259(11) 1.000 0.0243(12) . .
C211 C Uani 0.9109(2) 0.07584(19) 0.03442(10) 1.000 0.0250(12) . .
C212 C Uani 0.9358(2) 0.13835(19) 0.01248(11) 1.000 0.0256(11) . .
C213 C Uani 0.9524(2) 0.26914(19) 0.01766(11) 1.000 0.0245(11) . .
C214 C Uani 0.9425(2) 0.32869(19) 0.04525(11) 1.000 0.0245(11) . .
C215 C Uani 0.8980(2) 0.36510(19) 0.11569(11) 1.000 0.0253(12) . .
```

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C216 C Uani 0.8667(2) 0.33966(19) 0.15493(11) 1.000 0.0283(12) . .
C217 C Uani 0.8228(2) 0.2311(2) 0.19380(11) 1.000 0.0275(11) . .
C218 C Uani 0.8137(2) 0.1551(2) 0.19025(10) 1.000 0.0276(12) . .
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C226 C Uani 0.9316(3) 0.3287(2) 0.19031(11) 1.000 0.0274(12) . .
C227 C Uani 0.9051(3) 0.2619(2) 0.21377(11) 1.000 0.0277(12) . .
C228 C Uani 0.8874(3) 0.1085(2) 0.20720(11) 1.000 0.0270(12) . .
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C230 C Uani 0.9495(3) 0.00198(19) 0.09547(11) 1.000 0.0273(12) . .
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C233 C Uani 1.1222(3) 0.2675(2) 0.03226(11) 1.000 0.0313(12) . .
C234 C Uani 1.1118(2) 0.3298(2) 0.06081(11) 1.000 0.0283(12) . .
C235 C Uani 1.0585(3) 0.3737(2) 0.14525(11) 1.000 0.0297(12) . .
C236 C Uani 1.0261(3) 0.3461(2) 0.18636(11) 1.000 0.0307(12) . .
C237 C Uani 0.9745(3) 0.2171(2) 0.23221(11) 1.000 0.0317(14) . .
C238 C Uani 0.9648(3) 0.1376(2) 0.22899(11) 1.000 0.0307(14) . .
C239 C Uani 0.9861(2) 0.0141(2) 0.17260(11) 1.000 0.0294(12) . .
C240 C Uani 1.0122(2) -0.0085(2) 0.12990(11) 1.000 0.0283(12) . .
C241 C Uani 1.1415(2) 0.0363(2) 0.08582(12) 1.000 0.0323(12) . .
C242 C Uani 1.1841(2) 0.1434(2) 0.04737(12) 1.000 0.0329(14) . .
C243 C Uani 1.1943(3) 0.2194(2) 0.05091(12) 1.000 0.0323(14) . .
C244 C Uani 1.1767(2) 0.3213(2) 0.09690(12) 1.000 0.0303(12) . .
C245 C Uani 1.1510(3) 0.3422(2) 0.13825(12) 1.000 0.0314(12) . .
C246 C Uani 1.0973(3) 0.2984(2) 0.20484(11) 1.000 0.0318(12) . .
C247 C Uani 1.0723(3) 0.2346(2) 0.22728(11) 1.000 0.0331(14) . .
C248 C Uani 1.0566(3) 0.1063(2) 0.22198(11) 1.000 0.0311(12) . .
C249 C Uani 1.0673(2) 0.0457(2) 0.19453(11) 1.000 0.0308(12) . .
C250 C Uani 1.1102(2) 0.0103(2) 0.12509(12) 1.000 0.0313(12) . .
C251 C Uani 1.2076(2) 0.0966(2) 0.08445(12) 1.000 0.0330(12) . .
C252 C Uani 1.2278(2) 0.2527(2) 0.09060(12) 1.000 0.0320(12) . .
C253 C Uani 1.1748(3) 0.2959(2) 0.17524(12) 1.000 0.0354(14) . .
C254 C Uani 1.1229(3) 0.1665(2) 0.22121(11) 1.000 0.0345(14) . .
C255 C Uani 1.1440(3) 0.0427(2) 0.16497(12) 1.000 0.0334(12) . .
C256 C Uani 1.2416(2) 0.1281(2) 0.12288(13) 1.000 0.0360(16) . .
C257 C Uani 1.2508(2) 0.2083(2) 0.12629(13) 1.000 0.0341(16) . .
C258 C Uani 1.2241(3) 0.2302(2) 0.16915(12) 1.000 0.0358(14) . .
C259 C Uani 1.1974(3) 0.1638(2) 0.19265(12) 1.000 0.0348(14) . .
C260 C Uani 1.2082(2) 0.1014(2) 0.16426(12) 1.000 0.0331(12) . .
C261 C Uani 0.7422(2) 0.02384(19) 0.03674(11) 1.000 0.0256(12) . .
C262 C Uani 0.7205(3) 0.0352(2) -0.00628(12) 1.000 0.0330(12) . .
C263 C Uani 0.6509(3) -0.0035(2) -0.02700(12) 1.000 0.0350(14) . .
C264 C Uani 0.5994(3) -0.0573(2) -0.00617(12) 1.000 0.0335(12) . .
C265 C Uani 0.6170(3) -0.0660(2) 0.03766(13) 1.000 0.0431(17) . .
C266 C Uani 0.6878(3) -0.0260(2) 0.05875(12) 1.000 0.0428(16) . .
C267 C Uani 0.5299(3) -0.1050(2) -0.03117(13) 1.000 0.0421(16) . .
C268 C Uani 0.4927(3) -0.1710(2) -0.00806(14) 1.000 0.0505(17) . .
C269 C Uani 0.4442(3) -0.2259(2) -0.03783(14) 1.000 0.0530(17) . .
C270 C Uani 0.8238(3) 0.2182(2) -0.03363(11) 1.000 0.0276(12) . .
C271 C Uani 0.7523(3) 0.2695(2) -0.03719(12) 1.000 0.0350(14) . .
C272 C Uani 0.7018(3) 0.2781(2) -0.07589(12) 1.000 0.0401(16) . .
C273 C Uani 0.7211(3) 0.2342(2) -0.11196(12) 1.000 0.0404(16) . .
C274 C Uani 0.7921(3) 0.1834(2) -0.10822(12) 1.000 0.0387(16) . .
C275 C Uani 0.8442(3) 0.1758(2) -0.07000(11) 1.000 0.0337(14) . .
C276 C Uani 0.6645(3) 0.2421(3) -0.15394(14) 1.000 0.0578(17) . .
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C277 C Uani 0.5628(4) 0.2440(4) -0.14815(16) 1.000 0.086(3) . .
C278 C Uani 0.5261(3) 0.1809(3) -0.12510(16) 1.000 0.079(2) . .
C279 C Uani 0.7982(2) 0.40967(19) 0.05190(11) 1.000 0.0263(12) . .
C280 C Uani 0.7028(3) 0.4058(2) 0.04535(11) 1.000 0.0320(12) . .
C281 C Uani 0.6536(3) 0.4637(2) 0.02466(12) 1.000 0.0374(16) . .
C282 C Uani 0.7001(3) 0.5262(2) 0.01004(12) 1.000 0.0384(14) . .
C283 C Uani 0.7950(3) 0.5307(2) 0.01850(12) 1.000 0.0347(14) . .
C284 C Uani 0.8432(3) 0.4742(2) 0.03874(11) 1.000 0.0303(12) . .
C285 C Uani 0.6500(3) 0.5876(2) -0.01478(14) 1.000 0.0487(17) . .
C286 C Uani 0.6379(3) 0.6569(3) 0.01124(15) 1.000 0.0626(17) . .
C287 C Uani 0.5717(3) 0.6474(3) 0.04680(15) 1.000 0.0668(17) . .
C288 C Uani 0.6925(3) 0.32627(19) 0.17233(11) 1.000 0.0266(12) . .
C289 C Uani 0.6871(3) 0.3718(2) 0.20899(12) 1.000 0.0346(12) . .
C290 C Uani 0.6044(3) 0.4096(2) 0.21756(12) 1.000 0.0406(16) . .
C291 C Uani 0.5262(3) 0.4033(2) 0.19056(12) 1.000 0.0349(12) . .
C292 C Uani 0.5319(3) 0.3573(2) 0.15504(12) 1.000 0.0354(14) . .
C293 C Uani 0.6134(3) 0.3192(2) 0.14588(12) 1.000 0.0336(12) . .
C294 C Uani 0.4374(3) 0.4469(2) 0.19863(13) 1.000 0.0452(17) . .
C295 C Uani 0.4310(3) 0.5211(3) 0.17558(14) 1.000 0.0519(17) . .
C296 C Uani 0.4327(3) 0.5166(3) 0.12664(14) 1.000 0.066(2) . .
C297 C Uani 0.6684(2) 0.08128(19) 0.16537(11) 1.000 0.0259(11) . .
C298 C Uani 0.6657(3) 0.0276(2) 0.19818(11) 1.000 0.0317(12) . .
C299 C Uani 0.5830(3) -0.0069(2) 0.20883(12) 1.000 0.0356(14) . .
C2100 C Uani 0.5003(3) 0.0112(2) 0.18769(12) 1.000 0.0356(14) . .
C2101 C Uani 0.5029(3) 0.0640(2) 0.15557(12) 1.000 0.0347(14) . .
C2102 C Uani 0.5858(3) 0.0991(2) 0.14441(11) 1.000 0.0317(12) . .
C2103 C Uani 0.4099(3) -0.0252(2) 0.20112(13) 1.000 0.0443(16) . .
C2104 C Uani 0.3760(3) 0.0033(2) 0.24451(14) 1.000 0.0508(17) . .
C2105 C Uani 0.2860(3) -0.0336(3) 0.25816(15) 1.000 0.0655(19) . .


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H263 H Uiso 0.63750 0.00687 -0.05663 1.000 0.0417 . .
H265 H Uiso 0.58039 -0.09969 0.05374 1.000 0.0521 . .
H266 H Uiso 0.69874 -0.03333 0.08888 1.000 0.0511 . .
H267 H Uiso 0.47662 -0.07329 -0.04005 1.000 0.0503 . .
H267' H Uiso 0.55979 -0.12240 -0.05793 1.000 0.0503 . .
H268 H Uiso 0.44827 -0.15402 0.01397 1.000 0.0608 . .
H268' H Uiso 0.54470 -0.19632 0.00730 1.000 0.0608 . .
H269 H Uiso 0.39063 -0.20192 -0.05206 1.000 0.0793 . .
H269' H Uiso 0.42292 -0.26838 -0.02092 1.000 0.0793 . .
H269" H Uiso 0.48766 -0.24287 -0.05980 1.000 0.0793 . .
H271 H Uiso 0.73740 0.29927 -0.01290 1.000 0.0417 . .
H272 H Uiso 0.65376 0.31419 -0.07776 1.000 0.0481 . .
H274 H Uiso 0.80589 0.15271 -0.13227 1.000 0.0463 . .
H275 H Uiso 0.89421 0.14131 -0.06869 1.000 0.0405 . .
H276 H Uiso 0.68364 0.28824 -0.16863 1.000 0.0693 . .
H276' H Uiso 0.67969 0.20006 -0.17320 1.000 0.0693 . .
H277 H Uiso 0.54668 0.28967 -0.13221 1.000 0.1030 . .
H277' H Uiso 0.53189 0.24662 -0.17703 1.000 0.1030 . .
H278 H Uiso 0.55101 0.13506 -0.13741 1.000 0.1188 . .
H278' H Uiso 0.45808 0.18059 -0.12786 1.000 0.1188 . .
H278" H Uiso 0.54438 0.18421 -0.09444 1.000 0.1188 . .
H280 H Uiso 0.66992 0.36333 0.05498 1.000 0.0389 . .
H281 H Uiso 0.58810 0.45998 0.02065 1.000 0.0452 . .
H283 H Uiso 0.82764 0.57404 0.01011 1.000 0.0416 . .
H284 H Uiso 0.90827 0.47913 0.04383 1.000 0.0364 . .
H285 H Uiso 0.68570 0.59963 -0.04099 1.000 0.0585 . .
H285' H Uiso 0.58804 0.56946 -0.02438 1.000 0.0585 . .
H286 H Uiso 0.69905 0.67209 0.02355 1.000 0.0752 . .
H286' H Uiso 0.61545 0.69703 -0.00812 1.000 0.0752 . .
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H287' H Uiso 0.56933 0.69314 0.06389 1.000 0.1002 . .
H287" H Uiso 0.59221 0.60635 0.06544 1.000 0.1002 . .
H289 H Uiso 0.73942 0.37699 0.22797 1.000 0.0416 . .
H290 H Uiso 0.60163 0.44032 0.24248 1.000 0.0483 . .
H292 H Uiso 0.47901 0.35142 0.13645 1.000 0.0424 . .
H293 H Uiso 0.61520 0.28796 0.12116 1.000 0.0401 . .
H294 H Uiso 0.38349 0.41615 0.18937 1.000 0.0544 . .
H294' H Uiso 0.43237 0.45546 0.23016 1.000 0.0544 . .
H295 H Uiso 0.37275 0.54595 0.18410 1.000 0.0621 . .
H295' H Uiso 0.48357 0.55251 0.18566 1.000 0.0621 . .
H296 H Uiso 0.49314 0.49757 0.11761 1.000 0.0992 . .
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H298 H Uiso 0.72144 0.01460 0.21334 1.000 0.0380 . .
H299 H Uiso 0.58315 -0.04340 0.23098 1.000 0.0426 . .
H2101 H Uiso 0.44695 0.07702 0.14061 1.000 0.0419 . .
H2102 H Uiso 0.58518 0.13546 0.12218 1.000 0.0378 . .
H2103 H Uiso 0.41925 -0.07947 0.20301 1.000 0.0530 . .
H2103' H Uiso 0.36146 -0.01566 0.17859 1.000 0.0530 . .
H2104 H Uiso 0.42465 -0.00581 0.26698 1.000 0.0608 . .
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H2105' H Uiso 0.26704 -0.01350 0.28612 1.000 0.0980 . .
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C2101 0.024(2) 0.051(3) 0.029(2) 0.002(2) -0.0010(18) -0.0013(19)
C2102 0.029(2) 0.043(2) 0.023(2) 0.0060(19) -0.0022(18) -0.0039(19)
C2103 0.034(2) 0.052(3) 0.047(3) 0.012(2) 0.006(2) -0.007(2)
C2104 0.034(3) 0.064(3) 0.055(3) 0.017(2) 0.016(2) 0.003(2)
C2105 0.038(3) 0.097(4) 0.062(3) 0.035(3) 0.015(2) 0.008(3)
C21 0.022(2) 0.028(2) 0.0188(19) 0.0002(17) 0.0014(16) 0.0011(17)
C22 0.024(2) 0.031(2) 0.0163(19) -0.0022(17) -0.0003(16) 0.0017(17)
C23 0.019(2) 0.032(2) 0.020(2) 0.0022(18) -0.0005(16) 0.0012(17)
C24 0.021(2) 0.030(2) 0.019(2) -0.0019(17) -0.0005(16) -0.0001(16)
C25 0.0187(19) 0.032(2) 0.021(2) 0.0036(17) 0.0018(16) -0.0019(17)
C26 0.027(2) 0.033(2) 0.019(2) -0.0003(17) 0.0009(17) 0.0012(17)
C27 0.026(2) 0.033(2) 0.021(2) 0.0011(17) -0.0007(17) 0.0028(18)
C28 0.023(2) 0.032(2) 0.020(2) 0.0001(17) -0.0028(16) -0.0002(17)
C29 0.024(2) 0.035(2) 0.0166(19) 0.0002(17) 0.0006(16) -0.0018(17)
C210 0.020(2) 0.032(2) 0.021(2) 0.0001(17) 0.0018(16) -0.0026(17)
C211 0.028(2) 0.030(2) 0.017(2) -0.0043(17) 0.0005(17) 0.0018(18)
C212 0.029(2) 0.031(2) 0.0167(19) -0.0015(17) 0.0009(16) 0.0000(18)
C213 0.025(2) 0.032(2) 0.0166(19) 0.0045(17) 0.0008(16) 0.0003(17)
C214 0.027(2) 0.029(2) 0.0174(19) 0.0071(17) 0.0000(17) -0.0004(17)
C215 0.027(2) 0.025(2) 0.024(2) -0.0045(17) 0.0013(17) -0.0019(17)
C216 0.027(2) 0.033(2) 0.025(2) -0.0061(18) 0.0047(18) -0.0026(18)
C217 0.027(2) 0.042(2) 0.0138(19) -0.0019(18) 0.0061(17) -0.0027(19)
C218 0.023(2) 0.044(2) 0.016(2) 0.0034(18) 0.0064(16) -0.0028(19)
C219 0.021(2) 0.030(2) 0.023(2) 0.0050(17) -0.0006(17) -0.0029(17)
C220 0.023(2) 0.031(2) 0.023(2) -0.0005(17) 0.0002(17) -0.0013(17)
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C221 0.028(2) 0.028(2) 0.024(2) -0.0027(17) 0.0051(17) 0.0011(18)
C222 0.033(2) 0.040(2) 0.0148(19) -0.0001(18) 0.0069(17) -0.001(2)
C223 0.029(2) 0.036(2) 0.018(2) 0.0020(18) 0.0060(17) 0.0019(19)
C224 0.029(2) 0.028(2) 0.023(2) 0.0052(17) 0.0008(17) -0.0037(18)
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C226 0.030(2) 0.034(2) 0.018(2) -0.0052(18) -0.0030(17) -0.0068(18)
C227 0.029(2) 0.037(2) 0.017(2) -0.0015(18) 0.0004(18) -0.0030(19)
C228 0.030(2) 0.034(2) 0.017(2) 0.0037(18) 0.0004(17) -0.0022(19)
C229 0.028(2) 0.031(2) 0.021(2) 0.0066(17) 0.0011(18) -0.0020(18)
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C232 0.029(2) 0.033(2) 0.025(2) -0.0017(18) 0.0091(18) 0.0040(19)
C233 0.030(2) 0.039(2) 0.025(2) 0.0036(19) 0.0069(18) -0.004(2)
C234 0.026(2) 0.031(2) 0.028(2) 0.0052(18) 0.0069(18) -0.0060(18)
C235 0.031(2) 0.032(2) 0.026(2) -0.0017(18) -0.0012(19) -0.0047(18)
C236 0.034(2) 0.035(2) 0.023(2) -0.0045(18) -0.0041(18) -0.0068(19)
C237 0.034(2) 0.045(3) 0.016(2) -0.0007(19) 0.0014(18) -0.008(2)
C238 0.031(2) 0.045(3) 0.016(2) 0.0036(19) -0.0003(17) 0.000(2)
C239 0.028(2) 0.035(2) 0.025(2) 0.0107(18) -0.0052(18) 0.0004(18)
C240 0.025(2) 0.034(2) 0.026(2) 0.0045(18) 0.0001(18) 0.0018(18)
C241 0.025(2) 0.038(2) 0.034(2) 0.0016(19) 0.0030(19) 0.0054(19)
C242 0.021(2) 0.044(3) 0.034(2) 0.001(2) 0.0077(18) 0.0026(19)
C243 0.024(2) 0.043(3) 0.030(2) 0.006(2) 0.0069(18) 0.0014(19)
C244 0.022(2) 0.037(2) 0.032(2) 0.0042(19) 0.0003(18) -0.0085(18)
C245 0.027(2) 0.034(2) 0.033(2) 0.0006(19) -0.0031(18) -0.0072(18)
C246 0.031(2) 0.042(2) 0.022(2) -0.0028(19) -0.0074(18) -0.007(2)
C247 0.031(2) 0.047(3) 0.021(2) 0.0005(19) -0.0074(18) -0.004(2)
C248 0.030(2) 0.042(2) 0.021(2) 0.0071(19) -0.0095(17) -0.007(2)
C249 0.027(2) 0.040(2) 0.025(2) 0.0102(19) -0.0085(18) -0.0002(19)
C250 0.025(2) 0.032(2) 0.037(2) 0.0053(19) 0.0014(19) 0.0062(18)
C251 0.020(2) 0.041(2) 0.038(2) 0.003(2) 0.0019(19) 0.0054(19)
C252 0.022(2) 0.040(2) 0.034(2) 0.008(2) -0.0002(18) -0.0049(18)
C253 0.031(2) 0.044(3) 0.031(2) 0.002(2) -0.0066(19) -0.007(2)
C254 0.031(2) 0.051(3) 0.021(2) 0.0040(19) -0.0099(18) -0.005(2)
C255 0.030(2) 0.039(2) 0.031(2) 0.0073(19) -0.0076(19) 0.006(2)
C256 0.021(2) 0.047(3) 0.040(3) 0.007(2) -0.0002(19) 0.0037(19)
C257 0.018(2) 0.042(3) 0.042(3) 0.003(2) -0.0035(18) -0.0022(18)
C258 0.026(2) 0.049(3) 0.032(2) 0.007(2) -0.0061(18) -0.004(2)
C259 0.027(2) 0.044(3) 0.033(2) 0.008(2) -0.0128(18) -0.0018(19)
C260 0.021(2) 0.042(2) 0.036(2) 0.006(2) -0.0091(18) 0.0024(19)
C261 0.025(2) 0.028(2) 0.024(2) 0.0017(18) 0.0023(17) 0.0020(17)
C262 0.030(2) 0.042(2) 0.027(2) -0.0012(19) -0.0016(19) -0.0025(19)
C263 0.033(2) 0.049(3) 0.023(2) 0.001(2) -0.0021(19) 0.000(2)
C264 0.034(2) 0.036(2) 0.030(2) -0.0034(19) -0.0092(19) 0.002(2)
C265 0.050(3) 0.047(3) 0.032(3) 0.006(2) -0.008(2) -0.017(2)
C266 0.055(3) 0.049(3) 0.024(2) 0.002(2) -0.008(2) -0.013(2)
C267 0.039(3) 0.049(3) 0.038(2) 0.000(2) -0.006(2) -0.005(2)
C268 0.050(3) 0.051(3) 0.050(3) 0.003(2) -0.015(2) -0.010(2)
C269 0.060(3) 0.043(3) 0.055(3) 0.003(2) -0.022(2) -0.012(2)
C270 0.032(2) 0.030(2) 0.021(2) 0.0003(18) 0.0030(18) -0.0014(18)
C271 0.043(3) 0.039(2) 0.023(2) -0.0018(19) -0.0008(19) 0.003(2)
C272 0.041(3) 0.048(3) 0.031(2) 0.004(2) -0.007(2) 0.008(2)
C273 0.050(3) 0.051(3) 0.020(2) 0.001(2) -0.005(2) -0.005(2)
C274 0.053(3) 0.043(3) 0.020(2) -0.0004(19) 0.002(2) 0.003(2)
C275 0.044(3) 0.034(2) 0.023(2) 0.0041(19) 0.002(2) 0.0044(19)
C276 0.064(3) 0.074(3) 0.035(3) 0.000(2) -0.010(2) 0.002(3)
C277 0.080(4) 0.146(6) 0.032(3) -0.008(3) -0.001(3) 0.002(4)
C278 0.060(3) 0.120(5) 0.058(4) -0.011(3) 0.004(3) -0.028(3)
C279 0.026(2) 0.034(2) 0.019(2) -0.0001(17) 0.0017(16) 0.0026(18)
C280 0.034(2) 0.031(2) 0.031(2) 0.0015(19) -0.0006(19) -0.0010(19)
C281 0.029(2) 0.041(3) 0.042(3) 0.003(2) -0.0072(19) 0.001(2)

```
C282 0.044(3) 0.037(2) 0.034(2) 0.006(2) -0.003(2) 0.005(2)
C283 0.037(3) 0.031(2) 0.036(2) 0.0034(19) 0.000(2) -0.001(2)
C284 0.026(2) 0.033(2) 0.032(2) -0.0011(19) 0.0013(18) -0.0007(19)
C285 0.042(3) 0.048(3) 0.056(3) 0.006(2) -0.002(2) 0.006(2)
C286 0.064(3) 0.058(3) 0.066(3) 0.006(3) 0.004(3) 0.014(3)
C287 0.069(3) 0.064(3) 0.068(3) 0.010(3) 0.015(3) 0.021(3)
C288 0.029(2) 0.031(2) 0.020(2) -0.0025(18) 0.0035(18) -0.0012(18)
C289 0.031(2) 0.043(2) 0.030(2) -0.007(2) 0.0052(18) -0.003(2)
C290 0.046(3) 0.044(3) 0.032(2) -0.011(2) 0.010(2) -0.002(2)
C291 0.027(2) 0.044(2) 0.034(2) -0.003(2) 0.008(2) 0.000(2)
C292 0.029(2) 0.047(3) 0.030(2) -0.004(2) -0.0010(18) 0.004(2)
C293 0.037(2) 0.040(2) 0.024(2) -0.0063(19) 0.0039(19) 0.004(2)
C294 0.037(3) 0.054(3) 0.045(3) -0.013(2) 0.010(2) 0.008(2)
C295 0.040(3) 0.063(3) 0.053(3) -0.006(3) 0.006(2) 0.012(2)
C296 0.071(4) 0.073(4) 0.055(3) 0.003(3) 0.011(3) 0.020(3)
C297 0.031(2) 0.030(2) 0.0167(19) -0.0021(17) 0.0019(17) -0.0057(18)
C298 0.027(2) 0.042(2) 0.026(2) 0.0034(19) -0.0003(18) 0.0017(19)
C299 0.034(2) 0.045(3) 0.028(2) 0.0100(19) 0.0051(19) -0.001(2)
O11 0.053(2) 0.078(2) 0.0365(18) 0.0013(16) -0.0010(15) 0.0255(17)
O12 0.0498(19) 0.0524(19) 0.057(2) 0.0232(16) 0.0169(15) 0.0099(15)
O13 0.053(2) 0.089(2) 0.0335(18) -0.0028(17) 0.0061(15) -0.0007(18)
O14 0.066(2) 0.117(3) 0.039(2) -0.013(2) 0.0030(17) 0.002(2)
C11 0.062(3) 0.086(4) 0.052(3) -0.009(3) -0.002(3) 0.033(3)
C12 0.046(3) 0.095(4) 0.061(3) -0.020(3) -0.013(3) 0.019(3)
C13 0.044(3) 0.049(3) 0.039(3) 0.002(2) -0.005(2) -0.007(2)
C14 0.046(3) 0.057(3) 0.025(2) -0.003(2) 0.002(2) -0.001(2)
C15 0.051(3) 0.050(3) 0.052(3) 0.006(2) 0.023(2) 0.001(2)
C16 0.049(3) 0.075(4) 0.070(3) 0.022(3) 0.011(3) 0.002(3)
C17 0.058(3) 0.063(3) 0.041(3) 0.005(2) 0.006(2) 0.012(3)
C18 0.058(3) 0.054(3) 0.067(3) 0.027(3) 0.009(3) 0.005(3)
C19 0.064(3) 0.063(3) 0.029(3) 0.004(2) 0.010(2) 0.009(3)
C110 0.082(4) 0.056(3) 0.066(4) 0.015(3) 0.038(3) 0.017(3)
C111 0.063(4) 0.057(3) 0.091(4) -0.003(3) 0.005(3) 0.006(3)
C112 0.097(5) 0.117(5) 0.062(4) 0.011(4) -0.004(4) -0.015(4)
C113 0.089(4) 0.059(3) 0.068(4) 0.010(3) 0.006(3) 0.012(3)
C114 0.113(6) 0.078(4) 0.130(6) 0.004(4) -0.054(5) -0.028(4)
C115 0.264(12) 0.235(11) 0.197(10) 0.156(9) -0.177(9) -0.177(10)
C116 0.132(6) 0.227(9) 0.037(4) -0.026(5) 0.002(4) -0.023(6)
Li1 0.049(5) 0.085(6) 0.042(4) 0.021(4) -0.001(4) 0.015(4)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 O11     Li1        1.903(7)                    .       .                   yes
```

O11	C11	1.448(6)	.	.	yes
O11	C14	1.445(5)	.	.	yes
O12	C15	1.419(5)	.	.	yes
O12	C18	1.438(6)	.	.	yes
O12	Li1	1.902(8)	.	.	yes
O13	C19	1.427(5)	.	.	yes
O13	Li1	1.907(8)	.	.	yes
O13	C112	1.420(7)	.	.	yes
O14	Li1	1.917(9)	.	.	yes
O14	C116	1.426(7)	.	.	yes
O14	C113	1.467(6)	.	.	yes
C2100	C299	1.385(6)	.	.	no
C2100	C2103	1.521(6)	.	.	no
C2100	C2101	1.376(5)	.	.	no
C2101	C2102	1.398(6)	.	.	no
C2102	C297	1.380(5)	.	.	no
C2103	C2104	1.524(6)	.	.	no
C2104	C2105	1.522(6)	.	.	no
C21	C25	1.419(5)	.	.	no
C21	C22	1.404(5)	.	.	no
C21	C26	1.509(5)	.	.	no
C22	C27	1.515(5)	.	.	no
C22	C23	1.413(5)	.	.	no
C23	C28	1.515(5)	.	.	no
C23	C24	1.410(5)	.	.	no
C24	C25	1.410(5)	.	.	no
C24	C29	1.509(5)	.	.	no
C25	C210	1.510(5)	.	.	no
C26	C261	1.533(4)	.	.	no
C26	C211	1.559(4)	.	.	no
C26	C220	1.542(5)	.	.	no
C27	C212	1.540(5)	.	.	no
C27	C213	1.556(4)	.	.	no
C27	C270	1.531(5)	.	.	no
C28	C279	1.530(5)	.	.	no
C28	C215	1.543(5)	.	.	no
C28	C214	1.550(4)	.	.	no
C29	C216	1.547(4)	.	.	no
C29	C217	1.565(5)	.	.	no
C29	C288	1.539(5)	.	.	no
C2101	H2101	0.9500	.	.	no
C2102	H2102	0.9500	.	.	no
C2103	H2103'	0.9900	.	.	no
C2103	H2103	0.9900	.	.	no
C2104	H2104'	0.9900	.	.	no
C2104	H2104	0.9900	.	.	no
C2105	H2105"	0.9800	.	.	no
C2105	H2105'	0.9800	.	.	no
C2105	H2105	0.9800	.	.	no
C210	C297	1.541(4)	.	.	no
C210	C219	1.545(5)	.	.	no
C210	C218	1.546(5)	.	.	no
C211	C221	1.440(4)	.	.	no
C11	C12	1.482(6)	.	.	no
C211	C212	1.367(5)	.	.	no
C12	C13	1.531(6)	.	.	no
C212	C222	1.437(5)	.	.	no
C213	C223	1.430(5)	.	.	no
C213	C214	1.380(5)	.	.	no
C13	C14	1.519(6)	.	.	no
C214	C224	1.432(4)	.	.	no

C215	C216	1.379(5)	.	.	no
C215	C225	1.439(4)	.	.	no
C15	C16	1.485(6)	.	.	no
C216	C226	1.437(5)	.	.	no
C16	C17	1.531(7)	.	.	no
C217	C218	1.381(5)	.	.	no
C217	C227	1.436(5)	.	.	no
C17	C18	1.488(6)	.	.	no
C218	C228	1.443(5)	.	.	no
C219	C229	1.427(5)	.	.	no
C19	C110	1.510(7)	.	.	no
C219	C220	1.382(5)	.	.	no
C220	C230	1.444(5)	.	.	no
C221	C230	1.460(5)	.	.	no
C221	C231	1.399(5)	.	.	no
C222	C232	1.391(6)	.	.	no
C222	C223	1.471(5)	.	.	no
C223	C233	1.401(6)	.	.	no
C224	C225	1.449(5)	.	.	no
C224	C234	1.402(4)	.	.	no
C225	C235	1.390(5)	.	.	no
C226	C236	1.402(6)	.	.	no
C226	C227	1.460(5)	.	.	no
C227	C237	1.397(6)	.	.	no
C228	C229	1.446(5)	.	.	no
C228	C238	1.392(6)	.	.	no
C229	C239	1.404(4)	.	.	no
C230	C240	1.394(5)	.	.	no
C231	C241	1.461(5)	.	.	no
C231	C232	1.446(5)	.	.	no
C232	C242	1.453(5)	.	.	no
C233	C234	1.438(5)	.	.	no
C233	C243	1.462(6)	.	.	no
C234	C244	1.448(5)	.	.	no
C235	C245	1.466(6)	.	.	no
C235	C236	1.449(5)	.	.	no
C236	C246	1.446(6)	.	.	no
C237	C247	1.452(6)	.	.	no
C237	C238	1.444(5)	.	.	no
C238	C248	1.455(6)	.	.	no
C239	C249	1.455(4)	.	.	no
C239	C240	1.437(5)	.	.	no
C240	C250	1.459(4)	.	.	no
C241	C251	1.446(5)	.	.	no
C241	C250	1.383(5)	.	.	no
C242	C243	1.383(5)	.	.	no
C242	C251	1.457(5)	.	.	no
C243	C252	1.440(5)	.	.	no
C244	C245	1.388(5)	.	.	no
C244	C252	1.454(5)	.	.	no
C245	C253	1.451(5)	.	.	no
C246	C247	1.394(5)	.	.	no
C246	C253	1.455(6)	.	.	no
C247	C254	1.442(5)	.	.	no
C248	C254	1.445(6)	.	.	no
C248	C249	1.394(5)	.	.	no
C249	C255	1.446(5)	.	.	no
C250	C255	1.440(5)	.	.	no
C251	C256	1.396(5)	.	.	no
C252	C257	1.397(5)	.	.	no
C253	C258	1.395(5)	.	.	no

C254	C259	1.401(6)	.	.	no
C255	C260	1.405(5)	.	.	no
C256	C257	1.456(5)	.	.	no
C256	C260	1.456(5)	.	.	no
C257	C258	1.440(5)	.	.	no
C258	C259	1.456(5)	.	.	no
C259	C260	1.437(5)	.	.	no
C261	C262	1.374(5)	.	.	no
C261	C266	1.379(5)	.	.	no
C262	C263	1.369(6)	.	.	no
C263	C264	1.386(5)	.	.	no
C264	C265	1.381(5)	.	.	no
C264	C267	1.519(6)	.	.	no
C265	C266	1.399(6)	.	.	no
C267	C268	1.492(5)	.	.	no
C268	C269	1.513(6)	.	.	no
C270	C271	1.386(6)	.	.	no
C270	C275	1.395(5)	.	.	no
C271	C272	1.395(5)	.	.	no
C272	C273	1.399(5)	.	.	no
C273	C276	1.524(6)	.	.	no
C273	C274	1.375(6)	.	.	no
C274	C275	1.393(5)	.	.	no
C276	C277	1.477(7)	.	.	no
C277	C278	1.447(8)	.	.	no
C279	C280	1.384(5)	.	.	no
C279	C284	1.396(5)	.	.	no
C280	C281	1.408(5)	.	.	no
C281	C282	1.390(5)	.	.	no
C282	C285	1.521(5)	.	.	no
C282	C283	1.387(6)	.	.	no
C283	C284	1.376(5)	.	.	no
C285	C286	1.498(6)	.	.	no
C286	C287	1.477(6)	.	.	no
C288	C293	1.394(6)	.	.	no
C288	C289	1.402(5)	.	.	no
C289	C290	1.400(6)	.	.	no
C290	C291	1.392(6)	.	.	no
C291	C294	1.524(6)	.	.	no
C291	C292	1.379(5)	.	.	no
C292	C293	1.392(6)	.	.	no
C294	C295	1.518(6)	.	.	no
C295	C296	1.514(6)	.	.	no
C297	C298	1.403(5)	.	.	no
C298	C299	1.387(6)	.	.	no
C110	C111	1.520(7)	.	.	no
C11	H11	0.9900	.	.	no
C111	C112	1.487(8)	.	.	no
C11	H11'	0.9900	.	.	no
C12	H12'	0.9900	.	.	no
C12	H12	0.9900	.	.	no
C13	H13'	0.9900	.	.	no
C13	H13	0.9900	.	.	no
C113	C114	1.496(9)	.	.	no
C14	H14	0.9900	.	.	no
C14	H14'	0.9900	.	.	no
C114	C115	1.523(11)	.	.	no
C115	C116	1.385(13)	.	.	no
C15	H15'	0.9900	.	.	no
C15	H15	0.9900	.	.	no
C16	H16'	0.9900	.	.	no

C16	H16	0.9900	.	.	no
C17	H17	0.9900	.	.	no
C17	H17'	0.9900	.	.	no
C18	H18	0.9900	.	.	no
C18	H18'	0.9900	.	.	no
C19	H19'	0.9900	.	.	no
C19	H19	0.9900	.	.	no
C262	H262	0.9500	.	.	no
C263	H263	0.9500	.	.	no
C265	H265	0.9500	.	.	no
C266	H266	0.9500	.	.	no
C267	H267	0.9900	.	.	no
C267	H267'	0.9900	.	.	no
C268	H268	0.9900	.	.	no
C268	H268'	0.9900	.	.	no
C269	H269	0.9800	.	.	no
C269	H269"	0.9800	.	.	no
C269	H269'	0.9800	.	.	no
C271	H271	0.9500	.	.	no
C272	H272	0.9500	.	.	no
C274	H274	0.9500	.	.	no
C275	H275	0.9500	.	.	no
C276	H276	0.9900	.	.	no
C276	H276'	0.9900	.	.	no
C277	H277'	0.9900	.	.	no
C277	H277	0.9900	.	.	no
C278	H278'	0.9800	.	.	no
C278	H278"	0.9800	.	.	no
C278	H278	0.9800	.	.	no
C280	H280	0.9500	.	.	no
C281	H281	0.9500	.	.	no
C283	H283	0.9500	.	.	no
C284	H284	0.9500	.	.	no
C285	H285	0.9900	.	.	no
C285	H285'	0.9900	.	.	no
C286	H286	0.9900	.	.	no
C286	H286'	0.9900	.	.	no
C287	H287'	0.9800	.	.	no
C287	H287"	0.9800	.	.	no
C287	H287	0.9800	.	.	no
C289	H289	0.9500	.	.	no
C290	H290	0.9500	.	.	no
C292	H292	0.9500	.	.	no
C293	H293	0.9500	.	.	no
C294	H294'	0.9900	.	.	no
C294	H294	0.9900	.	.	no
C295	H295	0.9900	.	.	no
C295	H295'	0.9900	.	.	no
C296	H296"	0.9800	.	.	no
C296	H296	0.9800	.	.	no
C296	H296'	0.9800	.	.	no
C298	H298	0.9500	.	.	no
C299	H299	0.9500	.	.	no
C110	H110'	0.9900	.	.	no
C110	H110	0.9900	.	.	no
C111	H111'	0.9900	.	.	no
C111	H111	0.9900	.	.	no
C112	H112'	0.9900	.	.	no
C112	H112	0.9900	.	.	no
C113	H113'	0.9900	.	.	no
C113	H113	0.9900	.	.	no

```
 C114    H114'        0.9900                    .      .                 no
 C114    H114         0.9900                    .      .                 no
 C115    H115'        0.9900                    .      .                 no
 C115    H115         0.9900                    .      .                 no
 C116    H116'        0.9900                    .      .                 no
 C116    H116         0.9900                    .      .                 no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 C14     O11     Li1        132.3(3)              .      .      .          yes
 C11     O11     C14        107.0(3)              .      .      .          yes
 C11     O11     Li1        120.5(3)              .      .      .          yes
 C18     O12     Li1        128.7(3)              .      .      .          yes
 C15     O12     Li1        123.9(3)              .      .      .          yes
 C15     O12     C18        105.1(3)              .      .      .          yes
 C19     O13     C112       109.8(4)              .      .      .          yes
 C19     O13     Li1        130.3(3)              .      .      .          yes
 C112    O13     Li1        119.8(4)              .      .      .          yes
 C113    O14     Li1        123.8(3)              .      .      .          yes
 C113    O14     C116       104.6(4)              .      .      .          yes
 C116    O14     Li1        123.3(5)              .      .      .          yes
 C2103   C2100   C299       120.0(3)              .      .      .          no
 C2101   C2100   C299       117.9(4)              .      .      .          no
 C2101   C2100   C2103      122.0(4)              .      .      .          no
 C2100   C2101   C2102      121.7(4)              .      .      .          no
 C2101   C2102   C297       120.6(3)              .      .      .          no
 C2100   C2103   C2104      112.5(3)              .      .      .          no
 C2103   C2104   C2105      112.6(3)              .      .      .          no
 C25     C21     C26        123.8(3)              .      .      .          no
 C22     C21     C26        124.6(3)              .      .      .          no
 C22     C21     C25        108.3(3)              .      .      .          no
 C21     C22     C23        108.2(3)              .      .      .          no
 C21     C22     C27        124.0(3)              .      .      .          no
 C23     C22     C27        124.4(3)              .      .      .          no
 C22     C23     C24        107.7(3)              .      .      .          no
 C24     C23     C28        123.8(3)              .      .      .          no
 C22     C23     C28        124.3(3)              .      .      .          no
 C23     C24     C25        108.5(3)              .      .      .          no
 C23     C24     C29        124.4(3)              .      .      .          no
 C25     C24     C29        124.4(3)              .      .      .          no
 C21     C25     C24        107.4(3)              .      .      .          no
 C21     C25     C210       123.9(3)              .      .      .          no
 C24     C25     C210       124.7(3)              .      .      .          no
 C21     C26     C261       113.5(2)              .      .      .          no
 C211    C26     C220       100.2(2)              .      .      .          no
 C21     C26     C220       106.7(3)              .      .      .          no
 C21     C26     C211       106.0(3)              .      .      .          no
 C211    C26     C261       114.7(3)              .      .      .          no
 C220    C26     C261       114.6(3)              .      .      .          no
 C22     C27     C213       106.3(3)              .      .      .          no
 C212    C27     C270       113.7(3)              .      .      .          no
 C22     C27     C270       115.3(3)              .      .      .          no
 C212    C27     C213       100.3(2)              .      .      .          no
 C22     C27     C212       106.5(3)              .      .      .          no
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C213	C27	C270	113.5(3)	.	.	.	no
C214	C28	C279	111.7(3)	.	.	.	no
C23	C28	C214	106.3(3)	.	.	.	no
C23	C28	C215	106.6(3)	.	.	.	no
C215	C28	C279	111.9(3)	.	.	.	no
C214	C28	C215	100.1(2)	.	.	.	no
C23	C28	C279	118.5(2)	.	.	.	no
C24	C29	C217	106.4(3)	.	.	.	no
C24	C29	C216	106.5(3)	.	.	.	no
C24	C29	C288	114.0(3)	.	.	.	no
C216	C29	C217	100.2(2)	.	.	.	no
C216	C29	C288	113.6(3)	.	.	.	no
C217	C29	C288	115.0(3)	.	.	.	no
C2100	C2101	H2101	119.00	.	.	.	no
C2102	C2101	H2101	119.00	.	.	.	no
C297	C2102	H2102	120.00	.	.	.	no
C2101	C2102	H2102	120.00	.	.	.	no
C2104	C2103	H2103	109.00	.	.	.	no
C2100	C2103	H2103'	109.00	.	.	.	no
C2100	C2103	H2103	109.00	.	.	.	no
C2104	C2103	H2103'	109.00	.	.	.	no
H2103	C2103	H2103'	108.00	.	.	.	no
C2103	C2104	H2104	109.00	.	.	.	no
C2105	C2104	H2104'	109.00	.	.	.	no
H2104	C2104	H2104'	108.00	.	.	.	no
C2105	C2104	H2104	109.00	.	.	.	no
C2103	C2104	H2104'	109.00	.	.	.	no
C2104	C2105	H2105'	110.00	.	.	.	no
C2104	C2105	H2105	109.00	.	.	.	no
H2105	C2105	H2105"	109.00	.	.	.	no
C2104	C2105	H2105"	110.00	.	.	.	no
H2105	C2105	H2105'	109.00	.	.	.	no
H2105'	C2105	H2105"	109.00	.	.	.	no
C25	C210	C219	106.9(3)	.	.	.	no
C25	C210	C297	118.0(3)	.	.	.	no
C25	C210	C218	106.4(3)	.	.	.	no
C218	C210	C297	113.5(3)	.	.	.	no
C219	C210	C297	110.0(3)	.	.	.	no
C218	C210	C219	100.4(2)	.	.	.	no
C212	C211	C221	119.6(3)	.	.	.	no
C26	C211	C221	109.4(3)	.	.	.	no
O11	C11	C12	104.2(4)	.	.	.	yes
C26	C211	C212	124.2(3)	.	.	.	no
C27	C212	C222	110.3(3)	.	.	.	no
C211	C212	C222	119.2(3)	.	.	.	no
C11	C12	C13	104.8(4)	.	.	.	no
C27	C212	C211	124.2(3)	.	.	.	no
C27	C213	C214	124.0(3)	.	.	.	no
C214	C213	C223	119.3(3)	.	.	.	no
C12	C13	C14	104.9(3)	.	.	.	no
C27	C213	C223	109.9(3)	.	.	.	no
C28	C214	C213	124.3(3)	.	.	.	no
C28	C214	C224	109.8(3)	.	.	.	no
C213	C214	C224	119.7(3)	.	.	.	no
O11	C14	C13	105.4(3)	.	.	.	yes
C216	C215	C225	119.4(3)	.	.	.	no
C28	C215	C225	109.8(3)	.	.	.	no
C28	C215	C216	124.5(3)	.	.	.	no
O12	C15	C16	107.9(3)	.	.	.	yes
C29	C216	C215	123.4(3)	.	.	.	no
C29	C216	C226	110.2(3)	.	.	.	no

C215	C216	C226	119.7(3)	.	.	.	no
C15	C16	C17	105.1(3)	.	.	.	no
C16	C17	C18	102.4(4)	.	.	.	no
C29	C217	C218	123.4(3)	.	.	.	no
C29	C217	C227	109.5(3)	.	.	.	no
C218	C217	C227	119.6(3)	.	.	.	no
O12	C18	C17	105.4(4)	.	.	.	yes
C217	C218	C228	118.8(3)	.	.	.	no
C210	C218	C217	124.7(3)	.	.	.	no
C210	C218	C228	109.5(3)	.	.	.	no
O13	C19	C110	106.4(4)	.	.	.	yes
C220	C219	C229	120.4(3)	.	.	.	no
C210	C219	C220	123.4(3)	.	.	.	no
C210	C219	C229	109.9(3)	.	.	.	no
C219	C220	C230	118.6(3)	.	.	.	no
C26	C220	C219	124.3(3)	.	.	.	no
C26	C220	C230	110.6(3)	.	.	.	no
C230	C221	C231	119.2(3)	.	.	.	no
C211	C221	C230	109.4(3)	.	.	.	no
C211	C221	C231	121.5(3)	.	.	.	no
C212	C222	C223	108.2(3)	.	.	.	no
C223	C222	C232	119.2(4)	.	.	.	no
C212	C222	C232	122.6(3)	.	.	.	no
C213	C223	C222	108.6(3)	.	.	.	no
C222	C223	C233	119.5(3)	.	.	.	no
C213	C223	C233	121.8(3)	.	.	.	no
C225	C224	C234	120.1(3)	.	.	.	no
C214	C224	C225	108.8(3)	.	.	.	no
C214	C224	C234	121.4(3)	.	.	.	no
C215	C225	C224	108.7(3)	.	.	.	no
C215	C225	C235	121.6(3)	.	.	.	no
C224	C225	C235	119.9(3)	.	.	.	no
C216	C226	C236	121.3(3)	.	.	.	no
C227	C226	C236	119.4(4)	.	.	.	no
C216	C226	C227	108.6(3)	.	.	.	no
C217	C227	C237	121.9(3)	.	.	.	no
C226	C227	C237	119.3(4)	.	.	.	no
C217	C227	C226	109.1(3)	.	.	.	no
C218	C228	C238	122.0(3)	.	.	.	no
C229	C228	C238	119.9(4)	.	.	.	no
C218	C228	C229	108.6(3)	.	.	.	no
C219	C229	C239	121.0(3)	.	.	.	no
C228	C229	C239	120.3(3)	.	.	.	no
C219	C229	C228	109.1(3)	.	.	.	no
C220	C230	C221	107.8(3)	.	.	.	no
C220	C230	C240	121.7(3)	.	.	.	no
C221	C230	C240	120.2(3)	.	.	.	no
C232	C231	C241	108.1(3)	.	.	.	no
C221	C231	C241	120.4(3)	.	.	.	no
C221	C231	C232	118.9(3)	.	.	.	no
C231	C232	C242	108.3(3)	.	.	.	no
C222	C232	C242	120.7(3)	.	.	.	no
C222	C232	C231	118.1(4)	.	.	.	no
C223	C233	C243	120.8(3)	.	.	.	no
C223	C233	C234	118.8(3)	.	.	.	no
C234	C233	C243	107.7(3)	.	.	.	no
C233	C234	C244	108.4(3)	.	.	.	no
C224	C234	C233	118.9(3)	.	.	.	no
C224	C234	C244	120.0(3)	.	.	.	no
C225	C235	C245	120.0(3)	.	.	.	no
C236	C235	C245	107.7(3)	.	.	.	no

C225	C235	C236	119.0(4)	.	.	.	no
C235	C236	C246	108.3(3)	.	.	.	no
C226	C236	C235	118.8(3)	.	.	.	no
C226	C236	C246	120.8(3)	.	.	.	no
C227	C237	C238	118.6(4)	.	.	.	no
C227	C237	C247	121.1(3)	.	.	.	no
C238	C237	C247	107.5(3)	.	.	.	no
C237	C238	C248	108.0(3)	.	.	.	no
C228	C238	C237	118.9(4)	.	.	.	no
C228	C238	C248	120.0(3)	.	.	.	no
C240	C239	C249	108.5(3)	.	.	.	no
C229	C239	C249	119.8(3)	.	.	.	no
C229	C239	C240	119.1(3)	.	.	.	no
C230	C240	C239	119.0(3)	.	.	.	no
C239	C240	C250	107.3(3)	.	.	.	no
C230	C240	C250	120.2(3)	.	.	.	no
C250	C241	C251	120.4(3)	.	.	.	no
C231	C241	C251	107.7(3)	.	.	.	no
C231	C241	C250	120.1(3)	.	.	.	no
C232	C242	C251	107.6(3)	.	.	.	no
C243	C242	C251	119.3(3)	.	.	.	no
C232	C242	C243	121.0(3)	.	.	.	no
C242	C243	C252	120.9(3)	.	.	.	no
C233	C243	C242	118.9(3)	.	.	.	no
C233	C243	C252	108.1(3)	.	.	.	no
C245	C244	C252	119.9(3)	.	.	.	no
C234	C244	C252	107.9(3)	.	.	.	no
C234	C244	C245	120.0(3)	.	.	.	no
C235	C245	C244	119.9(3)	.	.	.	no
C244	C245	C253	120.3(3)	.	.	.	no
C235	C245	C253	108.0(3)	.	.	.	no
C236	C246	C253	108.4(3)	.	.	.	no
C236	C246	C247	120.0(4)	.	.	.	no
C247	C246	C253	119.6(3)	.	.	.	no
C246	C247	C254	120.2(4)	.	.	.	no
C237	C247	C246	119.4(4)	.	.	.	no
C237	C247	C254	108.7(3)	.	.	.	no
C238	C248	C254	108.1(3)	.	.	.	no
C249	C248	C254	119.9(3)	.	.	.	no
C238	C248	C249	120.4(3)	.	.	.	no
C239	C249	C248	119.6(3)	.	.	.	no
C239	C249	C255	107.8(3)	.	.	.	no
C248	C249	C255	120.5(3)	.	.	.	no
C240	C250	C241	119.9(3)	.	.	.	no
C241	C250	C255	120.2(3)	.	.	.	no
C240	C250	C255	108.6(3)	.	.	.	no
C241	C251	C242	108.4(3)	.	.	.	no
C241	C251	C256	120.1(3)	.	.	.	no
C242	C251	C256	120.3(3)	.	.	.	no
C244	C252	C257	119.7(3)	.	.	.	no
C243	C252	C257	120.2(3)	.	.	.	no
C243	C252	C244	107.9(3)	.	.	.	no
C246	C253	C258	120.5(3)	.	.	.	no
C245	C253	C246	107.7(3)	.	.	.	no
C245	C253	C258	119.7(3)	.	.	.	no
C248	C254	C259	119.8(3)	.	.	.	no
C247	C254	C259	120.3(3)	.	.	.	no
C247	C254	C248	107.7(4)	.	.	.	no
C249	C255	C250	107.8(3)	.	.	.	no
C250	C255	C260	120.3(3)	.	.	.	no
C249	C255	C260	119.4(3)	.	.	.	no

C251	C256	C257	119.7(3)	.	.	.	no
C251	C256	C260	119.7(3)	.	.	.	no
C257	C256	C260	107.2(3)	.	.	.	no
C256	C257	C258	108.3(3)	.	.	.	no
C252	C257	C258	120.3(3)	.	.	.	no
C252	C257	C256	119.5(3)	.	.	.	no
C253	C258	C257	120.1(3)	.	.	.	no
C253	C258	C259	119.5(4)	.	.	.	no
C257	C258	C259	108.0(3)	.	.	.	no
C254	C259	C258	119.8(3)	.	.	.	no
C254	C259	C260	120.3(3)	.	.	.	no
C258	C259	C260	107.9(3)	.	.	.	no
C255	C260	C259	120.2(3)	.	.	.	no
C255	C260	C256	119.4(3)	.	.	.	no
C256	C260	C259	108.5(3)	.	.	.	no
C262	C261	C266	116.9(3)	.	.	.	no
C26	C261	C262	121.9(3)	.	.	.	no
C26	C261	C266	121.1(3)	.	.	.	no
C261	C262	C263	121.8(3)	.	.	.	no
C262	C263	C264	122.2(4)	.	.	.	no
C265	C264	C267	122.7(3)	.	.	.	no
C263	C264	C265	116.4(4)	.	.	.	no
C263	C264	C267	120.9(3)	.	.	.	no
C264	C265	C266	121.1(4)	.	.	.	no
C261	C266	C265	121.4(3)	.	.	.	no
C264	C267	C268	116.6(3)	.	.	.	no
C267	C268	C269	113.4(4)	.	.	.	no
C271	C270	C275	118.0(3)	.	.	.	no
C27	C270	C275	122.5(3)	.	.	.	no
C27	C270	C271	119.5(3)	.	.	.	no
C270	C271	C272	121.0(3)	.	.	.	no
C271	C272	C273	120.8(4)	.	.	.	no
C272	C273	C276	120.9(4)	.	.	.	no
C274	C273	C276	121.2(4)	.	.	.	no
C272	C273	C274	117.9(4)	.	.	.	no
C273	C274	C275	121.6(3)	.	.	.	no
C270	C275	C274	120.7(4)	.	.	.	no
C273	C276	C277	114.4(4)	.	.	.	no
C276	C277	C278	114.3(5)	.	.	.	no
C28	C279	C284	120.6(3)	.	.	.	no
C280	C279	C284	117.6(3)	.	.	.	no
C28	C279	C280	121.8(3)	.	.	.	no
C279	C280	C281	121.1(3)	.	.	.	no
C280	C281	C282	120.6(4)	.	.	.	no
C281	C282	C283	117.6(4)	.	.	.	no
C281	C282	C285	121.9(4)	.	.	.	no
C283	C282	C285	120.5(3)	.	.	.	no
C282	C283	C284	121.8(4)	.	.	.	no
C279	C284	C283	121.2(4)	.	.	.	no
C282	C285	C286	113.3(4)	.	.	.	no
C285	C286	C287	112.7(4)	.	.	.	no
C289	C288	C293	118.0(4)	.	.	.	no
C29	C288	C293	119.2(3)	.	.	.	no
C29	C288	C289	122.7(3)	.	.	.	no
C288	C289	C290	119.9(4)	.	.	.	no
C289	C290	C291	121.8(3)	.	.	.	no
C292	C291	C294	120.2(4)	.	.	.	no
C290	C291	C292	117.8(4)	.	.	.	no
C290	C291	C294	122.0(3)	.	.	.	no
C291	C292	C293	121.4(4)	.	.	.	no
C288	C293	C292	121.1(3)	.	.	.	no

C291	C294	C295	115.0(3)	.	.	.	no
C294	C295	C296	114.8(4)	.	.	.	no
C2102	C297	C210	122.8(3)	.	.	.	no
C2102	C297	C298	117.7(3)	.	.	.	no
C210	C297	C298	119.5(3)	.	.	.	no
C297	C298	C299	121.1(4)	.	.	.	no
C2100	C299	C298	121.0(3)	.	.	.	no
C19	C110	C111	102.8(4)	.	.	.	no
O11	C11	H11'	111.00	.	.	.	no
C12	C11	H11	111.00	.	.	.	no
O11	C11	H11	111.00	.	.	.	no
C110	C111	C112	103.1(4)	.	.	.	no
H11	C11	H11'	109.00	.	.	.	no
C12	C11	H11'	111.00	.	.	.	no
C13	C12	H12	111.00	.	.	.	no
C13	C12	H12'	111.00	.	.	.	no
C11	C12	H12'	111.00	.	.	.	no
H12	C12	H12'	109.00	.	.	.	no
O13	C112	C111	107.7(4)	.	.	.	yes
C11	C12	H12	111.00	.	.	.	no
C14	C13	H13	111.00	.	.	.	no
C12	C13	H13	111.00	.	.	.	no
C12	C13	H13'	111.00	.	.	.	no
O14	C113	C114	106.2(4)	.	.	.	yes
H13	C13	H13'	109.00	.	.	.	no
C14	C13	H13'	111.00	.	.	.	no
O11	C14	H14	111.00	.	.	.	no
C113	C114	C115	100.3(6)	.	.	.	no
C13	C14	H14'	111.00	.	.	.	no
O11	C14	H14'	111.00	.	.	.	no
C13	C14	H14	111.00	.	.	.	no
H14	C14	H14'	109.00	.	.	.	no
C114	C115	C116	110.3(8)	.	.	.	no
H15	C15	H15'	108.00	.	.	.	no
O12	C15	H15	110.00	.	.	.	no
O12	C15	H15'	110.00	.	.	.	no
C16	C15	H15'	110.00	.	.	.	no
C16	C15	H15	110.00	.	.	.	no
H16	C16	H16'	109.00	.	.	.	no
C17	C16	H16	111.00	.	.	.	no
C17	C16	H16'	111.00	.	.	.	no
O14	C116	C115	108.0(6)	.	.	.	yes
C15	C16	H16'	111.00	.	.	.	no
C15	C16	H16	111.00	.	.	.	no
C16	C17	H17'	111.00	.	.	.	no
H17	C17	H17'	109.00	.	.	.	no
C18	C17	H17	111.00	.	.	.	no
C18	C17	H17'	111.00	.	.	.	no
C16	C17	H17	111.00	.	.	.	no
C17	C18	H18'	111.00	.	.	.	no
O12	C18	H18	111.00	.	.	.	no
O12	C18	H18'	111.00	.	.	.	no
H18	C18	H18'	109.00	.	.	.	no
C17	C18	H18	111.00	.	.	.	no
C110	C19	H19	110.00	.	.	.	no
C110	C19	H19'	110.00	.	.	.	no
O13	C19	H19'	110.00	.	.	.	no
H19	C19	H19'	109.00	.	.	.	no
O13	C19	H19	110.00	.	.	.	no
C263	C262	H262	119.00	.	.	.	no
C261	C262	H262	119.00	.	.	.	no

C262	C263	H263	119.00	.	.	.	no
C264	C263	H263	119.00	.	.	.	no
C266	C265	H265	119.00	.	.	.	no
C264	C265	H265	119.00	.	.	.	no
C261	C266	H266	119.00	.	.	.	no
C265	C266	H266	119.00	.	.	.	no
C264	C267	H267'	108.00	.	.	.	no
C264	C267	H267	108.00	.	.	.	no
C268	C267	H267'	108.00	.	.	.	no
C268	C267	H267	108.00	.	.	.	no
H267'	C267	H267	107.00	.	.	.	no
C267	C268	H268'	109.00	.	.	.	no
C269	C268	H268'	109.00	.	.	.	no
C269	C268	H268	109.00	.	.	.	no
H268'	C268	H268	108.00	.	.	.	no
C267	C268	H268	109.00	.	.	.	no
C268	C269	H269'	109.00	.	.	.	no
H269'	C269	H269"	110.00	.	.	.	no
H269'	C269	H269	109.00	.	.	.	no
C268	C269	H269	109.00	.	.	.	no
H269"	C269	H269	109.00	.	.	.	no
C268	C269	H269"	109.00	.	.	.	no
C272	C271	H271	119.00	.	.	.	no
C270	C271	H271	120.00	.	.	.	no
C271	C272	H272	120.00	.	.	.	no
C273	C272	H272	120.00	.	.	.	no
C275	C274	H274	119.00	.	.	.	no
C273	C274	H274	119.00	.	.	.	no
C274	C275	H275	120.00	.	.	.	no
C270	C275	H275	120.00	.	.	.	no
C277	C276	H276'	109.00	.	.	.	no
C277	C276	H276	109.00	.	.	.	no
C273	C276	H276'	109.00	.	.	.	no
H276'	C276	H276	108.00	.	.	.	no
C273	C276	H276	109.00	.	.	.	no
C278	C277	H277	109.00	.	.	.	no
C276	C277	H277'	109.00	.	.	.	no
C276	C277	H277	109.00	.	.	.	no
C278	C277	H277'	109.00	.	.	.	no
H277'	C277	H277	108.00	.	.	.	no
C277	C278	H278"	109.00	.	.	.	no
C277	C278	H278'	110.00	.	.	.	no
H278"	C278	H278	109.00	.	.	.	no
H278'	C278	H278"	109.00	.	.	.	no
H278'	C278	H278	109.00	.	.	.	no
C277	C278	H278	109.00	.	.	.	no
C281	C280	H280	119.00	.	.	.	no
C279	C280	H280	119.00	.	.	.	no
C280	C281	H281	120.00	.	.	.	no
C282	C281	H281	120.00	.	.	.	no
C282	C283	H283	119.00	.	.	.	no
C284	C283	H283	119.00	.	.	.	no
C283	C284	H284	119.00	.	.	.	no
C279	C284	H284	119.00	.	.	.	no
C282	C285	H285'	109.00	.	.	.	no
C286	C285	H285	109.00	.	.	.	no
C282	C285	H285	109.00	.	.	.	no
C286	C285	H285'	109.00	.	.	.	no
H285'	C285	H285	108.00	.	.	.	no
H286'	C286	H286	108.00	.	.	.	no
C287	C286	H286	109.00	.	.	.	no

C285	C286	H286'	109.00	.	.	.	no
C285	C286	H286	109.00	.	.	.	no
C287	C286	H286'	109.00	.	.	.	no
C286	C287	H287	109.00	.	.	.	no
H287'	C287	H287"	109.00	.	.	.	no
C286	C287	H287"	109.00	.	.	.	no
C286	C287	H287'	109.00	.	.	.	no
H287"	C287	H287	110.00	.	.	.	no
H287'	C287	H287	109.00	.	.	.	no
C290	C289	H289	120.00	.	.	.	no
C288	C289	H289	120.00	.	.	.	no
C289	C290	H290	119.00	.	.	.	no
C291	C290	H290	119.00	.	.	.	no
C293	C292	H292	119.00	.	.	.	no
C291	C292	H292	119.00	.	.	.	no
C292	C293	H293	119.00	.	.	.	no
C288	C293	H293	119.00	.	.	.	no
C291	C294	H294	108.00	.	.	.	no
C295	C294	H294'	109.00	.	.	.	no
H294'	C294	H294	107.00	.	.	.	no
C295	C294	H294	109.00	.	.	.	no
C291	C294	H294'	109.00	.	.	.	no
C296	C295	H295'	109.00	.	.	.	no
C294	C295	H295	109.00	.	.	.	no
H295'	C295	H295	108.00	.	.	.	no
C296	C295	H295	109.00	.	.	.	no
C294	C295	H295'	109.00	.	.	.	no
C295	C296	H296'	109.00	.	.	.	no
H296'	C296	H296"	109.00	.	.	.	no
H296"	C296	H296	109.00	.	.	.	no
C295	C296	H296"	109.00	.	.	.	no
C295	C296	H296	110.00	.	.	.	no
H296'	C296	H296	110.00	.	.	.	no
C297	C298	H298	119.00	.	.	.	no
C299	C298	H298	119.00	.	.	.	no
C298	C299	H299	119.00	.	.	.	no
C2100	C299	H299	120.00	.	.	.	no
C19	C110	H110'	111.00	.	.	.	no
C111	C110	H110'	111.00	.	.	.	no
C111	C110	H110	111.00	.	.	.	no
H110'	C110	H110	109.00	.	.	.	no
C19	C110	H110	111.00	.	.	.	no
C110	C111	H111	111.00	.	.	.	no
C112	C111	H111'	111.00	.	.	.	no
C110	C111	H111'	111.00	.	.	.	no
H111'	C111	H111	109.00	.	.	.	no
C112	C111	H111	111.00	.	.	.	no
C111	C112	H112	110.00	.	.	.	no
H112'	C112	H112	108.00	.	.	.	no
C111	C112	H112'	110.00	.	.	.	no
O13	C112	H112'	110.00	.	.	.	no
O13	C112	H112	110.00	.	.	.	no
O14	C113	H113	110.00	.	.	.	no
C114	C113	H113'	110.00	.	.	.	no
O14	C113	H113'	110.00	.	.	.	no
H113'	C113	H113	109.00	.	.	.	no
C114	C113	H113	110.00	.	.	.	no
C113	C114	H114'	112.00	.	.	.	no
C113	C114	H114	112.00	.	.	.	no
C115	C114	H114	112.00	.	.	.	no
H114'	C114	H114	110.00	.	.	.	no

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 C115    C114    H114'       112.00            .      .      .          no
 C116    C115    H115'       109.00            .      .      .          no
 C116    C115    H115        110.00            .      .      .          no
 H115'   C115    H115        108.00            .      .      .          no
 C114    C115    H115'       110.00            .      .      .          no
 C114    C115    H115        110.00            .      .      .          no
 C115    C116    H116'       110.00            .      .      .          no
 O14     C116    H116'       110.00            .      .      .          no
 O14     C116    H116        110.00            .      .      .          no
 H116'   C116    H116        108.00            .      .      .          no
 C115    C116    H116        110.00            .      .      .          no
 O11     Li1     O13       112.8(4)            .      .      .          yes
 O11     Li1     O14       100.3(4)            .      .      .          yes
 O12     Li1     O14       112.0(4)            .      .      .          yes
 O13     Li1     O14       116.3(4)            .      .      .          yes
 O12     Li1     O13       106.6(4)            .      .      .          yes
 O11     Li1     O12       108.6(3)            .      .      .          yes

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 C11     O11     Li1     O14        -57.3(5)     .      .      .      .   no
 C14     O11     Li1     O12         10.3(7)     .      .      .      .   no
 C14     O11     Li1     O13       -107.7(5)     .      .      .      .   no
 C14     O11     Li1     O14        127.9(4)     .      .      .      .   no
 C11     O11     C14     C13        -29.7(4)     .      .      .      .   no
 Li1     O11     C14     C13        145.6(4)     .      .      .      .   no
 C11     O11     Li1     O12       -174.9(4)     .      .      .      .   no
 C11     O11     Li1     O13         67.1(6)     .      .      .      .   no
 C14     O11     C11     C12         38.4(4)     .      .      .      .   no
 Li1     O11     C11     C12       -137.6(4)     .      .      .      .   no
 C15     O12     Li1     O11         64.8(5)     .      .      .      .   no
 C18     O12     C15     C16        -28.4(4)     .      .      .      .   no
 Li1     O12     C15     C16        135.8(4)     .      .      .      .   no
 C15     O12     C18     C17         38.8(4)     .      .      .      .   no
 Li1     O12     C18     C17       -124.4(4)     .      .      .      .   no
 C15     O12     Li1     O14        -45.1(5)     .      .      .      .   no
 C18     O12     Li1     O11       -134.9(4)     .      .      .      .   no
 C15     O12     Li1     O13       -173.4(3)     .      .      .      .   no
 C18     O12     Li1     O14        115.2(5)     .      .      .      .   no
 C18     O12     Li1     O13        -13.1(6)     .      .      .      .   no
 C112    O13     Li1     O11         38.8(6)     .      .      .      .   no
 C19     O13     Li1     O14        -21.0(7)     .      .      .      .   no
 C112    O13     C19     C110        12.3(5)     .      .      .      .   no
 Li1     O13     C19     C110      -172.4(4)     .      .      .      .   no
 C112    O13     Li1     O12        -80.4(5)     .      .      .      .   no
 C112    O13     Li1     O14        153.9(4)     .      .      .      .   no
 C19     O13     Li1     O12        104.8(5)     .      .      .      .   no
 C19     O13     Li1     O11       -136.1(4)     .      .      .      .   no
 C19     O13     C112    C111         8.5(6)     .      .      .      .   no
 Li1     O13     C112    C111      -167.4(4)     .      .      .      .   no
 Li1     O14     C113    C114      -115.2(5)     .      .      .      .   no
 C113    O14     C116    C115       -27.5(8)     .      .      .      .   no
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Li1	O14	C116	C115	121.6(7)	.	.	.	.	no
C113	O14	Li1	O11	-39.6(5)	.	.	.	.	no
C116	O14	C113	C114	33.7(6)	.	.	.	.	no
C116	O14	Li1	O11	177.1(4)	.	.	.	.	no
C116	O14	Li1	O12	-67.8(5)	.	.	.	.	no
C116	O14	Li1	O13	55.1(6)	.	.	.	.	no
C113	O14	Li1	O13	-161.6(4)	.	.	.	.	no
C113	O14	Li1	O12	75.4(5)	.	.	.	.	no
C2101	C2100	C299	C298	0.5(5)	.	.	.	.	no
C299	C2100	C2103	C2104	72.5(4)	.	.	.	.	no
C2103	C2100	C2101	C2102	177.8(3)	.	.	.	.	no
C299	C2100	C2101	C2102	-0.4(6)	.	.	.	.	no
C2101	C2100	C2103	C2104	-105.6(4)	.	.	.	.	no
C2103	C2100	C299	C298	-177.6(3)	.	.	.	.	no
C2100	C2101	C2102	C297	0.4(6)	.	.	.	.	no
C2101	C2102	C297	C298	-0.5(5)	.	.	.	.	no
C2101	C2102	C297	C210	176.3(3)	.	.	.	.	no
C2100	C2103	C2104	C2105	-179.5(3)	.	.	.	.	no
C26	C21	C25	C24	159.4(3)	.	.	.	.	no
C26	C21	C25	C210	1.1(5)	.	.	.	.	no
C22	C21	C25	C210	-159.1(3)	.	.	.	.	no
C25	C21	C26	C220	-26.0(4)	.	.	.	.	no
C25	C21	C26	C261	101.2(4)	.	.	.	.	no
C25	C21	C22	C27	159.6(3)	.	.	.	.	no
C22	C21	C26	C211	24.9(4)	.	.	.	.	no
C22	C21	C26	C220	131.0(3)	.	.	.	.	no
C22	C21	C26	C261	-101.8(3)	.	.	.	.	no
C25	C21	C26	C211	-132.1(3)	.	.	.	.	no
C22	C21	C25	C24	-0.8(3)	.	.	.	.	no
C25	C21	C22	C23	-0.1(3)	.	.	.	.	no
C26	C21	C22	C23	-160.1(3)	.	.	.	.	no
C26	C21	C22	C27	-0.4(5)	.	.	.	.	no
C21	C22	C23	C24	1.1(3)	.	.	.	.	no
C27	C22	C23	C24	-158.6(3)	.	.	.	.	no
C27	C22	C23	C28	-1.1(5)	.	.	.	.	no
C21	C22	C27	C212	-24.9(4)	.	.	.	.	no
C21	C22	C27	C213	-131.2(3)	.	.	.	.	no
C21	C22	C27	C270	102.2(4)	.	.	.	.	no
C23	C22	C27	C212	131.6(3)	.	.	.	.	no
C21	C22	C23	C28	158.5(3)	.	.	.	.	no
C23	C22	C27	C270	-101.3(4)	.	.	.	.	no
C23	C22	C27	C213	25.3(4)	.	.	.	.	no
C22	C23	C24	C29	160.3(3)	.	.	.	.	no
C28	C23	C24	C25	-159.2(3)	.	.	.	.	no
C22	C23	C28	C214	-24.3(4)	.	.	.	.	no
C22	C23	C28	C215	-130.4(3)	.	.	.	.	no
C28	C23	C24	C29	2.6(5)	.	.	.	.	no
C22	C23	C24	C25	-1.6(3)	.	.	.	.	no
C24	C23	C28	C215	23.5(4)	.	.	.	.	no
C22	C23	C28	C279	102.4(4)	.	.	.	.	no
C24	C23	C28	C214	129.7(3)	.	.	.	.	no
C24	C23	C28	C279	-103.7(4)	.	.	.	.	no
C23	C24	C29	C216	-27.0(4)	.	.	.	.	no
C25	C24	C29	C288	-102.0(4)	.	.	.	.	no
C23	C24	C25	C210	159.6(3)	.	.	.	.	no
C29	C24	C25	C21	-160.3(3)	.	.	.	.	no
C23	C24	C29	C217	-133.3(3)	.	.	.	.	no
C23	C24	C29	C288	99.0(4)	.	.	.	.	no
C25	C24	C29	C216	132.0(3)	.	.	.	.	no
C25	C24	C29	C217	25.7(4)	.	.	.	.	no
C23	C24	C25	C21	1.5(3)	.	.	.	.	no

C29	C24	C25	C210	-2.3(5)	.	.	.	no
C24	C25	C210	C219	-129.5(3)	.	.	.	no
C21	C25	C210	C297	-99.5(4)	.	.	.	no
C24	C25	C210	C218	-22.9(4)	.	.	.	no
C24	C25	C210	C297	106.0(4)	.	.	.	no
C21	C25	C210	C218	131.6(3)	.	.	.	no
C21	C25	C210	C219	25.0(4)	.	.	.	no
C21	C26	C220	C230	-126.1(3)	.	.	.	no
C21	C26	C261	C262	77.3(4)	.	.	.	no
C21	C26	C261	C266	-98.8(4)	.	.	.	no
C211	C26	C261	C262	-44.7(4)	.	.	.	no
C211	C26	C220	C230	-15.8(3)	.	.	.	no
C21	C26	C211	C212	-24.3(4)	.	.	.	no
C220	C26	C211	C212	-135.1(3)	.	.	.	no
C261	C26	C211	C212	101.7(4)	.	.	.	no
C21	C26	C211	C221	126.2(3)	.	.	.	no
C220	C26	C211	C221	15.4(3)	.	.	.	no
C261	C26	C211	C221	-107.8(3)	.	.	.	no
C261	C26	C220	C219	-101.5(4)	.	.	.	no
C211	C26	C261	C266	139.2(3)	.	.	.	no
C261	C26	C220	C230	107.4(3)	.	.	.	no
C220	C26	C261	C262	-159.8(3)	.	.	.	no
C220	C26	C261	C266	24.1(4)	.	.	.	no
C21	C26	C220	C219	25.0(4)	.	.	.	no
C211	C26	C220	C219	135.2(3)	.	.	.	no
C212	C27	C270	C275	-13.6(5)	.	.	.	no
C212	C27	C270	C271	165.5(3)	.	.	.	no
C212	C27	C213	C223	15.7(3)	.	.	.	no
C213	C27	C270	C271	-80.7(4)	.	.	.	no
C213	C27	C270	C275	100.2(4)	.	.	.	no
C22	C27	C270	C271	42.2(5)	.	.	.	no
C212	C27	C213	C214	-134.8(3)	.	.	.	no
C270	C27	C213	C214	103.7(4)	.	.	.	no
C270	C27	C212	C222	105.7(3)	.	.	.	no
C22	C27	C270	C275	-136.9(4)	.	.	.	no
C22	C27	C213	C214	-24.1(4)	.	.	.	no
C270	C27	C212	C211	-102.6(4)	.	.	.	no
C22	C27	C212	C211	25.4(4)	.	.	.	no
C22	C27	C213	C223	126.4(3)	.	.	.	no
C213	C27	C212	C211	135.9(3)	.	.	.	no
C22	C27	C212	C222	-126.3(3)	.	.	.	no
C213	C27	C212	C222	-15.7(3)	.	.	.	no
C270	C27	C213	C223	-105.9(3)	.	.	.	no
C23	C28	C215	C225	126.4(3)	.	.	.	no
C215	C28	C279	C280	-115.3(3)	.	.	.	no
C214	C28	C279	C284	-44.4(4)	.	.	.	no
C215	C28	C214	C224	-15.9(3)	.	.	.	no
C23	C28	C214	C224	-126.7(3)	.	.	.	no
C279	C28	C214	C224	102.6(3)	.	.	.	no
C215	C28	C279	C284	66.9(4)	.	.	.	no
C279	C28	C215	C225	-102.5(3)	.	.	.	no
C279	C28	C215	C216	106.1(4)	.	.	.	no
C214	C28	C215	C225	15.9(3)	.	.	.	no
C23	C28	C279	C280	9.4(5)	.	.	.	no
C23	C28	C214	C213	25.4(4)	.	.	.	no
C215	C28	C214	C213	136.2(3)	.	.	.	no
C279	C28	C214	C213	-105.3(4)	.	.	.	no
C214	C28	C279	C280	133.4(3)	.	.	.	no
C23	C28	C215	C216	-25.0(4)	.	.	.	no
C23	C28	C279	C284	-168.4(3)	.	.	.	no
C214	C28	C215	C216	-135.6(3)	.	.	.	no

C24	C29	C288	C293	1.1(5)	.	.	.	no
C288	C29	C216	C215	-100.9(4)	.	.	.	no
C24	C29	C216	C215	25.4(4)	.	.	.	no
C217	C29	C288	C289	60.5(4)	.	.	.	no
C288	C29	C217	C227	-107.7(3)	.	.	.	no
C288	C29	C216	C226	108.0(3)	.	.	.	no
C217	C29	C216	C215	136.0(3)	.	.	.	no
C24	C29	C217	C227	125.2(3)	.	.	.	no
C216	C29	C288	C293	123.3(3)	.	.	.	no
C217	C29	C288	C293	-122.1(3)	.	.	.	no
C216	C29	C288	C289	-54.2(4)	.	.	.	no
C24	C29	C288	C289	-176.4(3)	.	.	.	no
C288	C29	C217	C218	102.9(4)	.	.	.	no
C216	C29	C217	C227	14.5(3)	.	.	.	no
C217	C29	C216	C226	-15.1(3)	.	.	.	no
C216	C29	C217	C218	-134.9(3)	.	.	.	no
C24	C29	C216	C226	-125.7(3)	.	.	.	no
C24	C29	C217	C218	-24.2(4)	.	.	.	no
C219	C210	C218	C228	-14.8(3)	.	.	.	no
C218	C210	C219	C229	15.2(3)	.	.	.	no
C297	C210	C219	C220	103.3(4)	.	.	.	no
C218	C210	C219	C220	-136.9(3)	.	.	.	no
C219	C210	C297	C298	51.3(4)	.	.	.	no
C25	C210	C219	C220	-26.0(4)	.	.	.	no
C219	C210	C218	C217	135.4(3)	.	.	.	no
C218	C210	C297	C298	-60.2(4)	.	.	.	no
C25	C210	C219	C229	126.0(3)	.	.	.	no
C297	C210	C218	C228	102.6(3)	.	.	.	no
C25	C210	C218	C228	-126.0(3)	.	.	.	no
C25	C210	C218	C217	24.2(4)	.	.	.	no
C297	C210	C218	C217	-107.3(4)	.	.	.	no
C219	C210	C297	C2102	-125.4(3)	.	.	.	no
C297	C210	C219	C229	-104.7(3)	.	.	.	no
C218	C210	C297	C2102	123.0(4)	.	.	.	no
C25	C210	C297	C2102	-2.5(5)	.	.	.	no
C25	C210	C297	C298	174.3(3)	.	.	.	no
C212	C211	C221	C231	-3.4(5)	.	.	.	no
C212	C211	C221	C230	142.0(3)	.	.	.	no
C221	C211	C212	C27	-148.5(3)	.	.	.	no
O11	C11	C12	C13	-30.8(5)	.	.	.	no
C26	C211	C212	C222	148.5(3)	.	.	.	no
C26	C211	C221	C231	-155.4(3)	.	.	.	no
C221	C211	C212	C222	0.8(5)	.	.	.	no
C26	C211	C212	C27	-0.8(5)	.	.	.	no
C26	C211	C221	C230	-10.1(4)	.	.	.	no
C211	C212	C222	C232	2.3(5)	.	.	.	no
C211	C212	C222	C223	-142.7(3)	.	.	.	no
C27	C212	C222	C223	10.6(4)	.	.	.	no
C11	C12	C13	C14	13.0(5)	.	.	.	no
C27	C212	C222	C232	155.5(3)	.	.	.	no
C27	C213	C214	C224	148.3(3)	.	.	.	no
C27	C213	C214	C28	-1.3(5)	.	.	.	no
C223	C213	C214	C28	-149.2(3)	.	.	.	no
C12	C13	C14	O11	9.6(4)	.	.	.	no
C27	C213	C223	C222	-10.5(4)	.	.	.	no
C214	C213	C223	C222	141.6(3)	.	.	.	no
C27	C213	C223	C233	-155.5(3)	.	.	.	no
C223	C213	C214	C224	0.4(5)	.	.	.	no
C214	C213	C223	C233	-3.5(5)	.	.	.	no
C213	C214	C224	C234	3.1(5)	.	.	.	no
C213	C214	C224	C225	-142.9(3)	.	.	.	no

C28	C214	C224	C225	10.7(4)	.	.	.	no
C28	C214	C224	C234	156.6(3)	.	.	.	no
C216	C215	C225	C224	142.4(3)	.	.	.	no
C225	C215	C216	C29	-148.5(3)	.	.	.	no
O12	C15	C16	C17	7.4(5)	.	.	.	no
C216	C215	C225	C235	-3.4(5)	.	.	.	no
C28	C215	C225	C235	-156.5(3)	.	.	.	no
C28	C215	C216	C226	148.9(3)	.	.	.	no
C225	C215	C216	C226	0.0(5)	.	.	.	no
C28	C215	C225	C224	-10.8(4)	.	.	.	no
C28	C215	C216	C29	0.4(5)	.	.	.	no
C215	C216	C226	C227	-141.6(3)	.	.	.	no
C15	C16	C17	C18	15.4(5)	.	.	.	no
C215	C216	C226	C236	2.5(5)	.	.	.	no
C29	C216	C226	C236	154.9(3)	.	.	.	no
C29	C216	C226	C227	10.8(4)	.	.	.	no
C29	C217	C218	C228	147.0(3)	.	.	.	no
C227	C217	C218	C210	-147.1(3)	.	.	.	no
C218	C217	C227	C226	141.5(3)	.	.	.	no
C218	C217	C227	C237	-3.9(5)	.	.	.	no
C29	C217	C218	C210	-0.6(5)	.	.	.	no
C227	C217	C218	C228	0.6(5)	.	.	.	no
C29	C217	C227	C237	-154.6(3)	.	.	.	no
C16	C17	C18	O12	-32.9(5)	.	.	.	no
C29	C217	C227	C226	-9.2(4)	.	.	.	no
C210	C218	C228	C229	9.6(4)	.	.	.	no
C217	C218	C228	C229	-142.6(3)	.	.	.	no
C217	C218	C228	C238	3.5(5)	.	.	.	no
C210	C218	C228	C238	155.7(3)	.	.	.	no
C210	C219	C229	C239	-156.9(3)	.	.	.	no
O13	C19	C110	C111	-27.3(5)	.	.	.	no
C220	C219	C229	C228	142.5(3)	.	.	.	no
C210	C219	C229	C228	-10.5(4)	.	.	.	no
C220	C219	C229	C239	-3.9(5)	.	.	.	no
C210	C219	C220	C230	149.9(3)	.	.	.	no
C229	C219	C220	C230	0.7(5)	.	.	.	no
C210	C219	C220	C26	1.0(5)	.	.	.	no
C229	C219	C220	C26	-148.2(3)	.	.	.	no
C26	C220	C230	C221	10.9(4)	.	.	.	no
C26	C220	C230	C240	155.8(3)	.	.	.	no
C219	C220	C230	C240	2.9(5)	.	.	.	no
C219	C220	C230	C221	-142.0(3)	.	.	.	no
C211	C221	C230	C240	-145.9(3)	.	.	.	no
C231	C221	C230	C220	145.9(3)	.	.	.	no
C231	C221	C230	C240	0.4(5)	.	.	.	no
C211	C221	C230	C220	-0.4(4)	.	.	.	no
C211	C221	C231	C232	2.8(5)	.	.	.	no
C211	C221	C231	C241	140.1(3)	.	.	.	no
C230	C221	C231	C232	-139.2(3)	.	.	.	no
C230	C221	C231	C241	-2.0(5)	.	.	.	no
C212	C222	C232	C242	-139.6(4)	.	.	.	no
C212	C222	C223	C233	146.0(3)	.	.	.	no
C212	C222	C223	C213	0.0(4)	.	.	.	no
C223	C222	C232	C231	138.6(4)	.	.	.	no
C223	C222	C232	C242	1.7(5)	.	.	.	no
C212	C222	C232	C231	-2.8(5)	.	.	.	no
C232	C222	C223	C233	-0.3(5)	.	.	.	no
C232	C222	C223	C213	-146.3(3)	.	.	.	no
C213	C223	C233	C243	140.0(4)	.	.	.	no
C213	C223	C233	C234	3.1(5)	.	.	.	no
C222	C223	C233	C234	-138.3(4)	.	.	.	no

C222	C223	C233	C243	-1.5(5)	.	.	.	no
C234	C224	C225	C215	-146.5(3)	.	.	.	no
C234	C224	C225	C235	0.0(5)	.	.	.	no
C214	C224	C225	C235	146.5(3)	.	.	.	no
C225	C224	C234	C244	1.5(5)	.	.	.	no
C214	C224	C234	C233	-3.4(5)	.	.	.	no
C214	C224	C225	C215	0.0(4)	.	.	.	no
C214	C224	C234	C244	-140.8(3)	.	.	.	no
C225	C224	C234	C233	138.9(3)	.	.	.	no
C215	C225	C235	C236	4.1(5)	.	.	.	no
C215	C225	C235	C245	140.3(4)	.	.	.	no
C224	C225	C235	C236	-137.9(3)	.	.	.	no
C224	C225	C235	C245	-1.8(5)	.	.	.	no
C216	C226	C227	C217	-0.9(4)	.	.	.	no
C236	C226	C227	C237	0.7(5)	.	.	.	no
C216	C226	C227	C237	145.6(3)	.	.	.	no
C236	C226	C227	C217	-145.8(3)	.	.	.	no
C216	C226	C236	C246	-139.8(4)	.	.	.	no
C227	C226	C236	C235	138.7(3)	.	.	.	no
C227	C226	C236	C246	0.6(5)	.	.	.	no
C216	C226	C236	C235	-1.7(5)	.	.	.	no
C226	C227	C237	C247	-1.9(5)	.	.	.	no
C217	C227	C237	C247	140.1(4)	.	.	.	no
C217	C227	C237	C238	3.2(5)	.	.	.	no
C226	C227	C237	C238	-138.9(4)	.	.	.	no
C238	C228	C229	C219	-146.4(3)	.	.	.	no
C218	C228	C238	C237	-4.2(5)	.	.	.	no
C218	C228	C238	C248	-140.7(4)	.	.	.	no
C229	C228	C238	C237	138.2(4)	.	.	.	no
C229	C228	C238	C248	1.7(5)	.	.	.	no
C218	C228	C229	C239	147.1(3)	.	.	.	no
C238	C228	C229	C239	0.2(5)	.	.	.	no
C218	C228	C229	C219	0.6(4)	.	.	.	no
C219	C229	C239	C240	3.4(5)	.	.	.	no
C228	C229	C239	C240	-139.2(3)	.	.	.	no
C228	C229	C239	C249	-1.8(5)	.	.	.	no
C219	C229	C239	C249	140.9(3)	.	.	.	no
C220	C230	C240	C239	-3.4(5)	.	.	.	no
C221	C230	C240	C239	137.4(3)	.	.	.	no
C221	C230	C240	C250	1.7(5)	.	.	.	no
C220	C230	C240	C250	-139.0(4)	.	.	.	no
C221	C231	C232	C222	0.2(5)	.	.	.	no
C241	C231	C232	C242	-0.1(4)	.	.	.	no
C241	C231	C232	C222	-141.8(3)	.	.	.	no
C221	C231	C241	C251	-141.4(3)	.	.	.	no
C232	C231	C241	C250	142.9(4)	.	.	.	no
C221	C231	C241	C250	1.6(5)	.	.	.	no
C221	C231	C232	C242	141.9(3)	.	.	.	no
C232	C231	C241	C251	0.0(4)	.	.	.	no
C222	C232	C242	C251	140.7(3)	.	.	.	no
C231	C232	C242	C251	0.1(4)	.	.	.	no
C231	C232	C242	C243	-142.0(4)	.	.	.	no
C222	C232	C242	C243	-1.4(5)	.	.	.	no
C234	C233	C243	C252	-0.3(4)	.	.	.	no
C223	C233	C234	C224	0.3(5)	.	.	.	no
C234	C233	C243	C242	142.8(3)	.	.	.	no
C243	C233	C234	C224	-141.6(3)	.	.	.	no
C223	C233	C243	C252	-141.3(3)	.	.	.	no
C223	C233	C243	C242	1.8(5)	.	.	.	no
C223	C233	C234	C244	142.2(3)	.	.	.	no
C243	C233	C234	C244	0.2(4)	.	.	.	no

C224	C234	C244	C245	-1.1(5)	.	.	.	.	no
C233	C234	C244	C252	-0.1(4)	.	.	.	.	no
C224	C234	C244	C252	141.2(3)	.	.	.	.	no
C233	C234	C244	C245	-142.4(3)	.	.	.	.	no
C245	C235	C236	C226	-142.6(3)	.	.	.	.	no
C245	C235	C236	C246	0.2(4)	.	.	.	.	no
C225	C235	C236	C246	141.2(3)	.	.	.	.	no
C236	C235	C245	C253	-0.3(4)	.	.	.	.	no
C225	C235	C245	C244	2.2(5)	.	.	.	.	no
C236	C235	C245	C244	142.7(3)	.	.	.	.	no
C225	C235	C236	C226	-1.6(5)	.	.	.	.	no
C225	C235	C245	C253	-140.9(3)	.	.	.	.	no
C226	C236	C246	C247	-0.6(5)	.	.	.	.	no
C235	C236	C246	C247	-142.5(3)	.	.	.	.	no
C226	C236	C246	C253	141.9(3)	.	.	.	.	no
C235	C236	C246	C253	-0.1(4)	.	.	.	.	no
C247	C237	C238	C248	-0.1(4)	.	.	.	.	no
C247	C237	C238	C228	-141.4(3)	.	.	.	.	no
C238	C237	C247	C246	143.0(3)	.	.	.	.	no
C227	C237	C247	C246	1.9(5)	.	.	.	.	no
C227	C237	C238	C248	142.1(3)	.	.	.	.	no
C227	C237	C247	C254	-141.3(3)	.	.	.	.	no
C227	C237	C238	C228	0.8(5)	.	.	.	.	no
C238	C237	C247	C254	-0.2(4)	.	.	.	.	no
C237	C238	C248	C249	-142.7(3)	.	.	.	.	no
C228	C238	C248	C254	141.2(3)	.	.	.	.	no
C237	C238	C248	C254	0.4(4)	.	.	.	.	no
C228	C238	C248	C249	-2.0(5)	.	.	.	.	no
C229	C239	C249	C255	-141.3(3)	.	.	.	.	no
C240	C239	C249	C248	142.9(3)	.	.	.	.	no
C240	C239	C249	C255	0.2(4)	.	.	.	.	no
C229	C239	C240	C250	141.0(3)	.	.	.	.	no
C249	C239	C240	C230	-141.6(3)	.	.	.	.	no
C229	C239	C240	C230	0.2(5)	.	.	.	.	no
C249	C239	C240	C250	-0.8(4)	.	.	.	.	no
C229	C239	C249	C248	1.4(5)	.	.	.	.	no
C230	C240	C250	C255	141.4(3)	.	.	.	.	no
C230	C240	C250	C241	-2.1(5)	.	.	.	.	no
C239	C240	C250	C255	1.2(4)	.	.	.	.	no
C239	C240	C250	C241	-142.3(3)	.	.	.	.	no
C231	C241	C250	C240	0.5(5)	.	.	.	.	no
C231	C241	C251	C256	144.0(3)	.	.	.	.	no
C250	C241	C251	C242	-142.7(3)	.	.	.	.	no
C250	C241	C251	C256	1.2(5)	.	.	.	.	no
C231	C241	C251	C242	0.1(4)	.	.	.	.	no
C231	C241	C250	C255	-138.9(4)	.	.	.	.	no
C251	C241	C250	C240	138.7(3)	.	.	.	.	no
C251	C241	C250	C255	-0.6(5)	.	.	.	.	no
C232	C242	C243	C252	137.9(4)	.	.	.	.	no
C251	C242	C243	C233	-138.2(3)	.	.	.	.	no
C251	C242	C243	C252	0.1(5)	.	.	.	.	no
C232	C242	C243	C233	-0.4(5)	.	.	.	.	no
C232	C242	C251	C241	-0.2(4)	.	.	.	.	no
C232	C242	C251	C256	-143.9(3)	.	.	.	.	no
C243	C242	C251	C241	142.7(3)	.	.	.	.	no
C243	C242	C251	C256	-1.1(5)	.	.	.	.	no
C233	C243	C252	C244	0.2(4)	.	.	.	.	no
C233	C243	C252	C257	142.3(3)	.	.	.	.	no
C242	C243	C252	C257	0.1(5)	.	.	.	.	no
C242	C243	C252	C244	-142.0(4)	.	.	.	.	no
C245	C244	C252	C243	142.3(3)	.	.	.	.	no

C245	C244	C252	C257	-0.1(5)	.	.	.	.	no
C252	C244	C245	C235	-138.5(3)	.	.	.	.	no
C234	C244	C252	C257	-142.4(3)	.	.	.	.	no
C234	C244	C252	C243	-0.1(4)	.	.	.	.	no
C252	C244	C245	C253	-0.1(5)	.	.	.	.	no
C234	C244	C245	C253	137.8(4)	.	.	.	.	no
C234	C244	C245	C235	-0.7(5)	.	.	.	.	no
C244	C245	C253	C246	-142.5(4)	.	.	.	.	no
C244	C245	C253	C258	0.3(6)	.	.	.	.	no
C235	C245	C253	C246	0.3(4)	.	.	.	.	no
C235	C245	C253	C258	143.1(4)	.	.	.	.	no
C253	C246	C247	C254	0.0(6)	.	.	.	.	no
C253	C246	C247	C237	-138.9(4)	.	.	.	.	no
C247	C246	C253	C258	0.1(6)	.	.	.	.	no
C236	C246	C253	C245	-0.2(4)	.	.	.	.	no
C236	C246	C247	C237	-0.6(5)	.	.	.	.	no
C236	C246	C247	C254	138.3(4)	.	.	.	.	no
C236	C246	C253	C258	-142.6(4)	.	.	.	.	no
C247	C246	C253	C245	142.5(4)	.	.	.	.	no
C237	C247	C254	C248	0.5(4)	.	.	.	.	no
C237	C247	C254	C259	142.7(4)	.	.	.	.	no
C246	C247	C254	C248	-142.4(4)	.	.	.	.	no
C246	C247	C254	C259	-0.2(6)	.	.	.	.	no
C254	C248	C249	C239	-138.4(4)	.	.	.	.	no
C254	C248	C249	C255	-0.4(5)	.	.	.	.	no
C238	C248	C254	C247	-0.6(4)	.	.	.	.	no
C238	C248	C254	C259	-143.0(4)	.	.	.	.	no
C238	C248	C249	C239	0.4(5)	.	.	.	.	no
C238	C248	C249	C255	138.5(4)	.	.	.	.	no
C249	C248	C254	C259	0.4(5)	.	.	.	.	no
C249	C248	C254	C247	142.8(3)	.	.	.	.	no
C248	C249	C255	C250	-141.8(3)	.	.	.	.	no
C239	C249	C255	C260	142.6(3)	.	.	.	.	no
C248	C249	C255	C260	0.3(5)	.	.	.	.	no
C239	C249	C255	C250	0.6(4)	.	.	.	.	no
C240	C250	C255	C260	-142.8(4)	.	.	.	.	no
C241	C250	C255	C249	142.3(3)	.	.	.	.	no
C241	C250	C255	C260	0.7(5)	.	.	.	.	no
C240	C250	C255	C249	-1.1(4)	.	.	.	.	no
C241	C251	C256	C257	-137.7(3)	.	.	.	.	no
C242	C251	C256	C257	1.9(4)	.	.	.	.	no
C242	C251	C256	C260	137.9(3)	.	.	.	.	no
C241	C251	C256	C260	-1.8(5)	.	.	.	.	no
C243	C252	C257	C256	0.7(5)	.	.	.	.	no
C244	C252	C257	C258	0.0(5)	.	.	.	.	no
C244	C252	C257	C256	138.4(3)	.	.	.	.	no
C243	C252	C257	C258	-137.8(4)	.	.	.	.	no
C246	C253	C258	C257	137.7(4)	.	.	.	.	no
C246	C253	C258	C259	0.1(6)	.	.	.	.	no
C245	C253	C258	C259	-138.0(4)	.	.	.	.	no
C245	C253	C258	C257	-0.3(6)	.	.	.	.	no
C247	C254	C259	C258	0.3(6)	.	.	.	.	no
C247	C254	C259	C260	-137.9(4)	.	.	.	.	no
C248	C254	C259	C258	138.0(4)	.	.	.	.	no
C248	C254	C259	C260	-0.2(5)	.	.	.	.	no
C249	C255	C260	C259	-0.1(5)	.	.	.	.	no
C250	C255	C260	C259	137.2(4)	.	.	.	.	no
C250	C255	C260	C256	-1.2(5)	.	.	.	.	no
C249	C255	C260	C256	-138.6(3)	.	.	.	.	no
C257	C256	C260	C259	-0.2(4)	.	.	.	.	no
C251	C256	C257	C252	-1.7(4)	.	.	.	.	no

C260	C256	C257	C252	−142.5(3)	.	.	.	.	no
C257	C256	C260	C255	142.6(3)	.	.	.	.	no
C251	C256	C260	C259	−141.0(3)	.	.	.	.	no
C251	C256	C260	C255	1.8(5)	.	.	.	.	no
C251	C256	C257	C258	141.2(3)	.	.	.	.	no
C260	C256	C257	C258	0.4(4)	.	.	.	.	no
C256	C257	C258	C253	−142.4(4)	.	.	.	.	no
C252	C257	C258	C253	0.2(5)	.	.	.	.	no
C252	C257	C258	C259	142.1(3)	.	.	.	.	no
C256	C257	C258	C259	−0.4(4)	.	.	.	.	no
C257	C258	C259	C254	−142.5(4)	.	.	.	.	no
C253	C258	C259	C260	142.5(4)	.	.	.	.	no
C253	C258	C259	C254	−0.2(6)	.	.	.	.	no
C257	C258	C259	C260	0.3(4)	.	.	.	.	no
C258	C259	C260	C255	−142.5(4)	.	.	.	.	no
C258	C259	C260	C256	0.0(4)	.	.	.	.	no
C254	C259	C260	C256	142.5(3)	.	.	.	.	no
C254	C259	C260	C255	0.0(5)	.	.	.	.	no
C262	C261	C266	C265	3.3(5)	.	.	.	.	no
C26	C261	C262	C263	−179.2(3)	.	.	.	.	no
C266	C261	C262	C263	−2.9(6)	.	.	.	.	no
C26	C261	C266	C265	179.6(3)	.	.	.	.	no
C261	C262	C263	C264	−1.2(6)	.	.	.	.	no
C262	C263	C264	C267	−173.3(4)	.	.	.	.	no
C262	C263	C264	C265	4.9(6)	.	.	.	.	no
C263	C264	C265	C266	−4.4(6)	.	.	.	.	no
C267	C264	C265	C266	173.8(4)	.	.	.	.	no
C263	C264	C267	C268	167.8(4)	.	.	.	.	no
C265	C264	C267	C268	−10.3(6)	.	.	.	.	no
C264	C265	C266	C261	0.4(6)	.	.	.	.	no
C264	C267	C268	C269	−165.3(3)	.	.	.	.	no
C27	C270	C271	C272	−178.7(3)	.	.	.	.	no
C27	C270	C275	C274	177.1(3)	.	.	.	.	no
C271	C270	C275	C274	−2.0(6)	.	.	.	.	no
C275	C270	C271	C272	0.5(6)	.	.	.	.	no
C270	C271	C272	C273	1.1(6)	.	.	.	.	no
C271	C272	C273	C274	−1.0(6)	.	.	.	.	no
C271	C272	C273	C276	178.5(4)	.	.	.	.	no
C272	C273	C276	C277	−47.0(6)	.	.	.	.	no
C274	C273	C276	C277	132.5(5)	.	.	.	.	no
C276	C273	C274	C275	180.0(4)	.	.	.	.	no
C272	C273	C274	C275	−0.5(6)	.	.	.	.	no
C273	C274	C275	C270	2.1(6)	.	.	.	.	no
C273	C276	C277	C278	−55.6(6)	.	.	.	.	no
C28	C279	C280	C281	−175.5(3)	.	.	.	.	no
C284	C279	C280	C281	2.4(5)	.	.	.	.	no
C280	C279	C284	C283	−2.4(5)	.	.	.	.	no
C28	C279	C284	C283	175.5(3)	.	.	.	.	no
C279	C280	C281	C282	0.4(5)	.	.	.	.	no
C280	C281	C282	C283	−3.1(5)	.	.	.	.	no
C280	C281	C282	C285	176.3(3)	.	.	.	.	no
C281	C282	C283	C284	3.1(6)	.	.	.	.	no
C285	C282	C283	C284	−176.3(3)	.	.	.	.	no
C283	C282	C285	C286	−73.3(5)	.	.	.	.	no
C281	C282	C285	C286	107.3(4)	.	.	.	.	no
C282	C283	C284	C279	−0.3(6)	.	.	.	.	no
C282	C285	C286	C287	−68.8(5)	.	.	.	.	no
C293	C288	C289	C290	−1.2(5)	.	.	.	.	no
C29	C288	C293	C292	−176.3(3)	.	.	.	.	no
C289	C288	C293	C292	1.2(5)	.	.	.	.	no
C29	C288	C289	C290	176.2(3)	.	.	.	.	no

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 C288    C289    C290    C291         0.1(6)     .       .       .       .   no
 C289    C290    C291    C292         1.0(6)     .       .       .       .   no
 C289    C290    C291    C294      -177.3(3)     .       .       .       .   no
 C290    C291    C292    C293        -1.0(6)     .       .       .       .   no
 C294    C291    C292    C293       177.3(3)     .       .       .       .   no
 C292    C291    C294    C295       -86.3(5)     .       .       .       .   no
 C290    C291    C294    C295        92.0(5)     .       .       .       .   no
 C291    C292    C293    C288        -0.1(6)     .       .       .       .   no
 C291    C294    C295    C296        61.2(5)     .       .       .       .   no
 C210    C297    C298    C299      -176.2(3)     .       .       .       .   no
 C2102   C297    C298    C299         0.7(5)     .       .       .       .   no
 C297    C298    C299    C2100       -0.7(6)     .       .       .       .   no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 O11     O12        3.089(4)                    .       .                   no
 O11     O13        3.173(4)                    .       .                   no
 O11     O14        2.933(4)                    .       .                   no
 O11     C113       3.304(6)                    .       .                   no
 O12     O11        3.089(4)                    .       .                   no
 O12     O13        3.054(4)                    .       .                   no
 O12     O14        3.166(4)                    .       .                   no
 O13     O12        3.054(4)                    .       .                   no
 O13     O11        3.173(4)                    .       .                   no
 O14     C11        3.386(5)                    .       .                   no
 O14     O11        2.933(4)                    .       .                   no
 O14     O12        3.166(4)                    .       .                   no
 O11     H113'        2.8000                    .       .                   no
 O13     H18'         2.8900                    .       .                   no
 C2104   C112       3.567(7)                    .       .                   no
 C2105   C294       3.518(6)                    .     2_545                 no
 C11     C113       3.600(7)                    .       .                   no
 C12     C259       3.565(6)                    .     1_455                 no
 C12     C258       3.400(6)                    .     1_455                 no
 C13     C292       3.592(5)                    .       .                   no
 C13     C258       3.287(6)                    .     1_455                 no
 C13     C259       3.515(6)                    .     1_455                 no
 C18     C215       3.549(6)                    .     2_645                 no
 C23     C271       3.597(5)                    .       .                   no
 C2100   H14          2.9900                    .       .                   no
 C2101   H14          3.0400                    .       .                   no
 C2101   H13          3.0700                    .       .                   no
 C2103   H278         2.8600                    .     3_655                 no
 C2104   H112         3.0500                    .       .                   no
 C2105   H294         3.0900                    .     2_545                 no
 C112    C2104      3.567(7)                    .       .                   no
 C13     H2104'       3.1000                    .       .                   no
 C113    C11        3.600(7)                    .       .                   no
 C115    C266      3.568(10)                    .     2_655                 no
 C16     H295'        3.0000                    .     2_645                 no
 C21     H269         2.8500                    .     3_655                 no
 C22     H269         2.9700                    .     3_655                 no
 C22     H271         2.7400                    .       .                   no
 C23     H293         3.0900                    .       .                   no
 C23     H271         2.9700                    .       .                   no
 C23     H280         2.6400                    .       .                   no
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C24	H293	2.4300	.	.	no
C25	H293	3.0700	.	.	no
C25	H269	2.9800	.	3_655	no
C25	H2102	2.6500	.	.	no
C211	C231	3.395(5)	.	3_755	no
C112	H2104	3.0300	.	.	no
C113	H15	3.0800	.	.	no
C114	H278'	2.9300	.	4_555	no
C114	H266	3.0500	.	2_655	no
C114	H15	3.0200	.	.	no
C215	C18	3.549(6)	.	2_655	no
C219	C266	3.600(5)	.	.	no
C221	C221	3.554(5)	.	3_755	no
C221	C231	3.555(5)	.	3_755	no
C224	C284	3.427(5)	.	.	no
C225	C284	3.525(5)	.	.	no
C228	C298	3.512(6)	.	.	no
C229	C298	3.423(5)	.	.	no
C231	C211	3.395(5)	.	3_755	no
C231	C221	3.555(5)	.	3_755	no
C231	C262	3.542(6)	.	3_755	no
C241	C263	3.572(5)	.	3_755	no
C241	C262	3.437(5)	.	3_755	no
C242	C263	3.528(5)	.	3_755	no
C248	C295	3.519(6)	.	2_645	no
C251	C263	3.200(5)	.	3_755	no
C251	C262	3.556(5)	.	3_755	no
C258	C12	3.400(6)	.	1_655	no
C258	C13	3.287(6)	.	1_655	no
C259	C12	3.565(6)	.	1_655	no
C259	C13	3.515(6)	.	1_655	no
C262	C251	3.556(5)	.	3_755	no
C262	C241	3.437(5)	.	3_755	no
C262	C231	3.542(6)	.	3_755	no
C263	C251	3.200(5)	.	3_755	no
C263	C242	3.528(5)	.	3_755	no
C263	C241	3.572(5)	.	3_755	no
C264	C264	3.553(6)	.	3_655	no
C266	C219	3.600(5)	.	.	no
C266	C115	3.568(10)	.	2_645	no
C271	C23	3.597(5)	.	.	no
C272	C278	3.409(6)	.	.	no
C278	C272	3.409(6)	.	.	no
C281	C287	3.587(6)	.	.	no
C284	C225	3.525(5)	.	.	no
C284	C224	3.427(5)	.	.	no
C287	C281	3.587(6)	.	.	no
C292	C296	3.319(6)	.	.	no
C292	C13	3.592(5)	.	.	no
C294	C2105	3.518(6)	.	2_555	no
C295	C248	3.519(6)	.	2_655	no
C296	C292	3.319(6)	.	.	no
C298	C229	3.423(5)	.	.	no
C298	C228	3.512(6)	.	.	no
C211	H262	2.8200	.	.	no
C212	H275	2.5700	.	.	no
C212	H262	3.0500	.	.	no
C213	H19	3.0100	.	4_554	no
C214	H284	2.7600	.	.	no
C215	H284	3.0300	.	.	no
C215	H18'	3.0100	.	2_655	no

C216	H18	3.0500	.	2_655	no
C216	H289	3.0100	.	.	no
C217	H289	3.0900	.	.	no
C218	H15'	2.8900	.	.	no
C218	H298	2.9500	.	.	no
C219	H266	2.9700	.	.	no
C219	H298	2.8000	.	.	no
C220	H266	2.5900	.	.	no
C222	H116	2.9200	.	4_554	no
C223	H116	2.9300	.	4_554	no
C224	H284	2.8200	.	.	no
C224	H110'	3.0200	.	2_655	no
C225	H284	2.9900	.	.	no
C228	H15'	3.0100	.	.	no
C228	H298	2.9300	.	.	no
C229	H290	3.1000	.	2_645	no
C229	H298	2.8300	.	.	no
C230	H113	3.1000	.	2_645	no
C234	H283	2.9400	.	3_765	no
C235	H112	2.9900	.	2_655	no
C237	H277'	2.9800	.	4_555	no
C239	H113	3.0400	.	2_645	no
C240	H113	2.9900	.	2_645	no
C244	H285	3.0100	.	3_765	no
C246	H2105"	2.7700	.	2_655	no
C247	H277'	3.0400	.	4_555	no
C248	H294'	3.1000	.	2_645	no
C248	H295'	3.0800	.	2_645	no
C249	H2105	3.0100	.	1_655	no
C249	H294'	2.8400	.	2_645	no
C251	H263	3.0400	.	3_755	no
C253	H2105"	2.9100	.	2_655	no
C255	H2105	2.8300	.	1_655	no
C258	H12	3.1000	.	1_655	no
C258	H13	2.9600	.	1_655	no
C259	H13	2.8800	.	1_655	no
C260	H2103'	3.0800	.	1_655	no
C264	H267	2.9700	.	3_655	no
C265	H115'	2.8000	.	2_645	no
C265	H268	2.9800	.	.	no
C265	H268'	2.7300	.	.	no
C265	H267	2.8500	.	3_655	no
C266	H267	3.0100	.	3_655	no
C266	H115'	2.7000	.	2_645	no
C266	H114	3.0800	.	2_645	no
C268	H265	2.6100	.	.	no
C268	H286'	2.9600	.	1_545	no
C269	H293	2.9200	.	3_655	no
C269	H286'	2.9600	.	1_545	no
C269	H280	3.0100	.	3_655	no
C269	H2102	3.1000	.	3_655	no
C270	H262	2.8600	.	.	no
C270	H19	2.7500	.	4_554	no
C271	H19	2.9700	.	4_554	no
C271	H110	3.0600	.	4_554	no
C272	H277	2.8100	.	.	no
C272	H111'	2.8700	.	4_554	no
C272	H278"	2.8800	.	.	no
C273	H278"	2.7600	.	.	no
C274	H11'	2.9500	.	4_554	no
C275	H19	2.9500	.	4_554	no

C275	H262	2.7400	.	.	no
C277	H272	2.8200	.	.	no
C278	H265	3.0800	.	3_655	no
C279	H271	2.9400	.	.	no
C280	H271	2.6900	.	.	no
C281	H287"	3.0000	.	.	no
C282	H287"	2.7400	.	.	no
C283	H286	2.9100	.	.	no
C283	H110	3.0100	.	4_554	no
C284	H110	2.9400	.	4_554	no
C286	H268'	2.9700	.	1_565	no
C287	H268'	3.0900	.	1_565	no
C287	H115	3.0900	.	2_655	no
C288	H17	3.0700	.	2_655	no
C288	H14'	3.0400	.	.	no
C289	H17	2.9400	.	2_655	no
C290	H17	3.0700	.	2_655	no
C290	H16'	2.9500	.	2_655	no
C291	H296	2.8600	.	.	no
C291	H13'	3.0900	.	.	no
C292	H296	2.8300	.	.	no
C292	H13'	2.7200	.	.	no
C293	H14'	3.0900	.	.	no
C293	H280	3.0400	.	.	no
C294	H2105'	3.0700	.	2_555	no
C296	H292	3.0700	.	.	no
C298	H15'	2.9900	.	.	no
C299	H14	3.0500	.	.	no
C299	H2104	2.9300	.	.	no
H110'	C224	3.0200	.	2_645	no
H111'	C272	2.8700	.	4_455	no
H113'	O11	2.8000	.	.	no
H114'	H15	2.3500	.	.	no
H114'	H278'	2.5400	.	4_555	no
H115'	C266	2.7000	.	2_655	no
H115'	C265	2.8000	.	2_655	no
H115'	H266	2.5300	.	2_655	no
H267'	H269"	2.4100	.	.	no
H267'	H263	2.5900	.	.	no
H268'	C265	2.7300	.	.	no
H268'	C286	2.9700	.	1_545	no
H268'	C287	3.0900	.	1_545	no
H268'	H286'	2.2300	.	1_545	no
H268'	H265	2.3100	.	.	no
H269'	H280	2.4000	.	3_655	no
H11'	C274	2.9500	.	4_455	no
H11'	H274	2.4800	.	4_455	no
H269"	H293	2.5200	.	3_655	no
H269"	H267'	2.4100	.	.	no
H12	C258	3.1000	.	1_455	no
H276'	H278	2.4700	.	.	no
H276'	H274	2.3500	.	.	no
H13	C258	2.9600	.	1_455	no
H13	C259	2.8800	.	1_455	no
H13	H2104'	2.2900	.	.	no
H13	C2101	3.0700	.	.	no
H13'	C291	3.0900	.	.	no
H13'	C292	2.7200	.	.	no
H277'	C237	2.9800	.	4_454	no
H277'	C247	3.0400	.	4_454	no
H14	C2100	2.9900	.	.	no

H14	C299	3.0500	.	.	no
H14	C2101	3.0400	.	.	no
H14'	C293	3.0900	.	.	no
H14'	C288	3.0400	.	.	no
H278'	C114	2.9300	.	4_454	no
H278'	H114'	2.5400	.	4_454	no
H15	C113	3.0800	.	.	no
H15	C114	3.0200	.	.	no
H15	H114'	2.3500	.	.	no
H15'	C218	2.8900	.	.	no
H15'	C228	3.0100	.	.	no
H15'	C298	2.9900	.	.	no
H278"	H268	2.5400	.	3_655	no
H278"	C272	2.8800	.	.	no
H278"	C273	2.7600	.	.	no
H16'	H295'	2.3600	.	2_645	no
H16'	C290	2.9500	.	2_645	no
H285'	H287	2.4800	.	.	no
H285'	H281	2.5900	.	3_665	no
H285'	H281	2.4200	.	.	no
H17	C290	3.0700	.	2_645	no
H17	C288	3.0700	.	2_645	no
H17	C289	2.9400	.	2_645	no
H17'	H287"	2.5400	.	2_645	no
H286'	C268	2.9600	.	1_565	no
H286'	H268'	2.2300	.	1_565	no
H286'	C269	2.9600	.	1_565	no
H18	C216	3.0500	.	2_645	no
H18'	O13	2.8900	.	.	no
H18'	C215	3.0100	.	2_645	no
H287'	H115	2.4600	.	2_655	no
H19	C213	3.0100	.	4_455	no
H19	C270	2.7500	.	4_455	no
H19	C271	2.9700	.	4_455	no
H19	C275	2.9500	.	4_455	no
H287"	C282	2.7400	.	.	no
H287"	H17'	2.5400	.	2_655	no
H287"	C281	3.0000	.	.	no
H294'	H290	2.4700	.	.	no
H294'	C249	2.8400	.	2_655	no
H294'	C248	3.1000	.	2_655	no
H295'	C16	3.0000	.	2_655	no
H295'	C248	3.0800	.	2_655	no
H295'	H16'	2.3600	.	2_655	no
H296"	H294	2.5600	.	.	no
H2101	H2103'	2.3900	.	.	no
H2102	C25	2.6500	.	.	no
H2102	C269	3.1000	.	3_655	no
H2102	H269	2.5100	.	3_655	no
H2103	H299	2.5800	.	.	no
H2103	H278	2.3100	.	3_655	no
H2103	H2105"	2.5400	.	.	no
H2103'	C260	3.0800	.	1_455	no
H2103'	H2101	2.3900	.	.	no
H2103'	H2105	2.5500	.	.	no
H2104	C112	3.0300	.	.	no
H2104	C299	2.9300	.	.	no
H2104	H112	2.3300	.	.	no
H2104'	H13	2.2900	.	.	no
H2104'	C13	3.1000	.	.	no
H2105	H2103'	2.5500	.	.	no

H2105	C249	3.0100	.	1_455	no
H2105	C255	2.8300	.	1_455	no
H2105'	H295	2.4700	.	2_545	no
H2105'	C294	3.0700	.	2_545	no
H2105"	C246	2.7700	.	2_645	no
H2105"	C253	2.9100	.	2_645	no
H2105"	H2103	2.5400	.	.	no
H110	C284	2.9400	.	4_455	no
H110	C283	3.0100	.	4_455	no
H110	C271	3.0600	.	4_455	no
H112	H2104	2.3300	.	.	no
H112	C235	2.9900	.	2_645	no
H112	C2104	3.0500	.	.	no
H113	C230	3.1000	.	2_655	no
H113	C239	3.0400	.	2_655	no
H113	C240	2.9900	.	2_655	no
H114	H266	2.2600	.	2_655	no
H114	C266	3.0800	.	2_655	no
H115	C287	3.0900	.	2_645	no
H115	H287'	2.4600	.	2_645	no
H115	H286	2.5800	.	2_645	no
H116	C222	2.9200	.	4_455	no
H116	C223	2.9300	.	4_455	no
H262	C211	2.8200	.	.	no
H262	C270	2.8600	.	.	no
H262	C275	2.7400	.	.	no
H262	C212	3.0500	.	.	no
H263	H267'	2.5900	.	.	no
H263	C251	3.0400	.	3_755	no
H265	C268	2.6100	.	.	no
H265	H268'	2.3100	.	.	no
H265	H268	2.4500	.	.	no
H265	C278	3.0800	.	3_655	no
H266	C219	2.9700	.	.	no
H266	H115'	2.5300	.	2_645	no
H266	H114	2.2600	.	2_645	no
H266	C114	3.0500	.	2_645	no
H266	C220	2.5900	.	.	no
H267	C265	2.8500	.	3_655	no
H267	C264	2.9700	.	3_655	no
H267	C266	3.0100	.	3_655	no
H268	H265	2.4500	.	.	no
H268	C265	2.9800	.	.	no
H268	H278"	2.5400	.	3_655	no
H269	C22	2.9700	.	3_655	no
H269	C21	2.8500	.	3_655	no
H269	C25	2.9800	.	3_655	no
H269	H2102	2.5100	.	3_655	no
H271	C279	2.9400	.	.	no
H271	C22	2.7400	.	.	no
H271	C23	2.9700	.	.	no
H271	C280	2.6900	.	.	no
H271	H280	2.6000	.	.	no
H272	C277	2.8200	.	.	no
H272	H277	2.3000	.	.	no
H274	H276'	2.3500	.	.	no
H274	H11'	2.4800	.	4_554	no
H275	C212	2.5700	.	.	no
H277	C272	2.8100	.	.	no
H277	H272	2.3000	.	.	no
H278	H276'	2.4700	.	.	no

H278	C2103	2.8600	.	3_655	no
H278	H2103	2.3100	.	3_655	no
H280	H269'	2.4000	.	3_655	no
H280	C23	2.6400	.	.	no
H280	C293	3.0400	.	.	no
H280	C269	3.0100	.	3_655	no
H280	H293	2.5900	.	.	no
H280	H271	2.6000	.	.	no
H281	H285'	2.4200	.	.	no
H281	H285'	2.5900	.	3_665	no
H283	H286	2.6000	.	.	no
H283	H285	2.6000	.	.	no
H283	C234	2.9400	.	3_765	no
H284	C214	2.7600	.	.	no
H284	C215	3.0300	.	.	no
H284	C225	2.9900	.	.	no
H284	C224	2.8200	.	.	no
H285	H283	2.6000	.	.	no
H285	C244	3.0100	.	3_765	no
H286	H283	2.6000	.	.	no
H286	H115	2.5800	.	2_655	no
H286	C283	2.9100	.	.	no
H287	H285'	2.4800	.	.	no
H289	C216	3.0100	.	.	no
H289	C217	3.0900	.	.	no
H290	C229	3.1000	.	2_655	no
H290	H294'	2.4700	.	.	no
H292	C296	3.0700	.	.	no
H292	H294	2.4500	.	.	no
H293	C23	3.0900	.	.	no
H293	C25	3.0700	.	.	no
H293	H280	2.5900	.	.	no
H293	C269	2.9200	.	3_655	no
H293	H269"	2.5200	.	3_655	no
H293	C24	2.4300	.	.	no
H294	H296"	2.5600	.	.	no
H294	H292	2.4500	.	.	no
H294	C2105	3.0900	.	2_555	no
H295	H2105'	2.4700	.	2_555	no
H296	C291	2.8600	.	.	no
H296	C292	2.8300	.	.	no
H298	C219	2.8000	.	.	no
H298	C218	2.9500	.	.	no
H298	C228	2.9300	.	.	no
H298	C229	2.8300	.	.	no
H299	H2103	2.5800	.	.	no

#===END of Crystallographic Information File